PATENT COOPERATION TREATY

PCT

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

(PCT Article 36 and Rule 70)

Applicant's or agent's file reference	FOR FURTHER ACTION	See Notification of Transmittal of International Preliminary Examination Report (Form PCT/IPEA/416)
P174-PCT11		
International application No.	International filing date *(day/month/year)*	Priority date *(day/month/year)*
PCT/CA00/00725	16/06/2000	18/06/1999
International Patent Classification (IPC) or national classification and IPC		
C12N9/10		
Applicant		
RINI, James et al.		

1. This international preliminary examination report has been prepared by this International Preliminary Examining Authority and is transmitted to the applicant according to Article 36.

2. This REPORT consists of a total of 7 sheets, including this cover sheet.

   ☐ This report is also accompanied by ANNEXES, i.e. sheets of the description, claims and/or drawings which have been amended and are the basis for this report and/or sheets containing rectifications made before this Authority (see Rule 70.16 and Section 607 of the Administrative Instructions under the PCT).

   These annexes consist of a total of sheets.

3. This report contains indications relating to the following items:

   - I ☒ Basis of the report
   - II ☐ Priority
   - III ☒ Non-establishment of opinion with regard to novelty, inventive step and industrial applicability
   - IV ☐ Lack of unity of invention
   - V ☒ Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations suporting such statement
   - VI ☐ Certain documents cited
   - VII ☐ Certain defects in the international application
   - VIII ☒ Certain observations on the international application

Date of submission of the demand	Date of completion of this report
18/01/2001	02.10.2001
Name and mailing address of the international preliminary examining authority:	Authorized officer
European Patent Office D-80298 Munich Tel. +49 89 2399 - 0 Tx: 523656 epmu d Fax: +49 89 2399 - 4465	Strobel, A Telephone No. +49 89 2399 7362

Form PCT/IPEA/409 (cover sheet) (January 1994)

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/CA00/00725

I. Basis of the report

1. With regard to the **elements** of the international application *(Replacement sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred to in this report as "originally filed" and are not annexed to this report since they do not contain amendments (Rules 70.16 and 70.17))*:
Description, pages:

1-245 as originally filed

Claims, No.:

1-35 as originally filed

Drawings, sheets:

1/53-53/53 as originally filed

Sequence listing part of the description, pages:

1, as originally filed

2. With regard to the **language**, all the elements marked above were available or furnished to this Authority in the language in which the international application was filed, unless otherwise indicated under this item.

These elements were available or furnished to this Authority in the following language: , which is:

- ☐ the language of a translation furnished for the purposes of the international search (under Rule 23.1(b)).
- ☐ the language of publication of the international application (under Rule 48.3(b)).
- ☐ the language of a translation furnished for the purposes of international preliminary examination (under Rule 55.2 and/or 55.3).

3. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application, the international preliminary examination was carried out on the basis of the sequence listing:

- ☒ contained in the international application in written form.
- ☐ filed together with the international application in computer readable form.
- ☐ furnished subsequently to this Authority in written form.
- ☒ furnished subsequently to this Authority in computer readable form.
- ☒ The statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.
- ☒ The statement that the information recorded in computer readable form is identical to the written sequence listing has been furnished.

4. The amendments have resulted in the cancellation of:

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/CA00/00725

- ☐ the description, pages:
- ☐ the claims, Nos.:
- ☐ the drawings, sheets:

5. ☐ This report has been established as if (some of) the amendments had not been made, since they have been considered to go beyond the disclosure as filed (Rule 70.2(c)):

   (Any replacement sheet containing such amendments must be referred to under item 1 and annexed to this report.)

6. Additional observations, if necessary:

III. Non-establishment of opinion with regard to novelty, inventive step and industrial applicability

1. The questions whether the claimed invention appears to be novel, to involve an inventive step (to be non-obvious), or to be industrially applicable have not been examined in respect of:

   ☐ the entire international application.

   ☒ claims Nos. 20, 27, 29-32 all partially, 34, 35 completely.

because:

   ☒ the said international application, or the said claims Nos. 34 and 35 relate to the following subject matter which does not require an international preliminary examination (*specify*):
   see separate sheet

   ☐ the description, claims or drawings (*indicate particular elements below*) or said claims Nos. are so unclear that no meaningful opinion could be formed (*specify*):

   ☐ the claims, or said claims Nos. are so inadequately supported by the description that no meaningful opinion could be formed.

   ☒ no international search report has been established for the said claims Nos. 20, 27, 29-32 all partially.

2. A meaningful international preliminary examination cannot be carried out due to the failure of the nucleotide and/or amino acid sequence listing to comply with the standard provided for in Annex C of the Administrative Instructions:

   ☐ the written form has not been furnished or does not comply with the standard.

   ☐ the computer readable form has not been furnished or does not comply with the standard.

V. Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/CA00/00725

1. Statement

Novelty (N)	Yes:	Claims	
	No:	Claims	1-7, 11, 13-16, 18-20, 27, 29
Inventive step (IS)	Yes:	Claims	
	No:	Claims	1-33
Industrial applicability (IA)	Yes:	Claims	1-30
	No:	Claims	

2. Citations and explanations
see separate sheet

VIII. Certain observations on the international application

The following observations on the clarity of the claims, description, and drawings or on the question whether the claims are fully supported by the description, are made:
see separate sheet

For reasons of better comprehension, the present opinion does not stick to the usual division into points I.-VIII.

Claims 1-10 and 14-19 are directed to two- or three-dimensional structures. The claims are therefore not directed to the product per se but only to the strucural information of the product. These claims are neither product claims nor method claims but appear to be mere presentation of information. The subject-matter of these claims is therefore, in principle, excluded from examination under Article 34(4)(a)(1) in combination with Rule 67.1(v) PCT.

Nevertheless, the following comments on novelty, inventive step, and clarity have been made:

Reference is made to the following documents:

D1: CHARNOCK SIMON J ET AL: 'Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms.' BIOCHEMISTRY, vol. 38, no. 20, 18 May 1999 (1999-05-18), pages 6380-6385

D2: NISHIKAWA Y ET AL: 'CONTROL OF GLYCOPROTEIN SYNTHESIS PURIFICATION AND CHARACTERIZATION OF RABBIT LIVER UDP-N-ACETYLGLUCOSAMINE ALPHA-3-D-MANNOSIDE BETA-1 2-N ACETYLGLUCOSAMINYLTRANSFERASE I' JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 263, no. 17, 1988, pages 8270-8281

D3: ULLMAN C AND PERKINS S: 'A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities' BIOCHEMICAL JOURNAL, vol. 326, 1997, pages 929-941

D4: KUNTZ I D ET AL: "STRUCTURE-BASED MOLECULAR DESIGN" ACCOUNTS OF CHEMICAL RESEARCH,US,AMERICAN CHEMICAL SOCIETY. WASHINGTON, vol. 27, no. 5, May 1994 (1994-05), pages 117-123

D5: GSCHWEND D A ET AL: "MOLECULAR DOCKING TOWARDS DRUG DISCOVERY" JOURNAL OF MOLECULAR RECOGNITION,GB,HEYDEN & SON LTD., LONDON, vol. 9, 1996, pages 175-186

1. Claims 20, 27, 29-32 have only been searched partially. Claims or parts of claims that have only been searched partially need not be the subject of an international preliminary examination, Rule 66.1(e) PCT. Thus, said claims are only examined with respect to UDP-GlcNAc.

Claims 34 and 35 concern the mere presentation of information and are thus

excluded from examination according to Rule 67.1(v) PCT.

2. **Clarity and Novelty**

Claims 1-7, 11, 13-16, and 18-33 do not fulfil the requirements of Article 6 PCT. The reasons for this lack of clarity are as follows:

Product claims 1-7, 11, 13-16, 18 and 19 directed to structures of glycosyltransferases (GT) do not define said structures at all or in a way that permits the man skilled in the art to clearly comprehend the subject-matter claimed. Said claims are so broad that they also are not novel over D1-3 which describe glycosyltransferases in solution or in crystal form as well as bound to substrates (Non-fulfilment of Article 33(2) PCT).

All claims directed to modulators, inhibitors of GT or methods for obtaining such modulators or inhibitors, namely claims 20, 22-33 are not supported by the description since, apart from the natural substrate UDP-GlcNAc, neither such compounds are disclosed nor are methods indicated that allow for the obtention of such compounds (i.e. the applicants actually do not provide any experimental data. If on the other hand the general and vague description of the claimed methods is sufficient for the obtention of such a compound, then said methods and compounds would certainly not be inventive). Of course, this objections holds also for the medical use of such hypothetical modulators, as defined in claims 31-33.

Claim 21 in its broadness lacks a recognisable technical problem and is therefor unclear.

Product claims have to be novel as such. D2 describes UDP-GlcNAc as a ligand of GTn-1. Thus, claims 20, 27, and 29 lack novelty (Article 33(2) PCT).

3. **Inventive step of claims 8-10, 12, 17, 21-26, 28, and 30-33**

Claims 8-10, 12 and 17 define structures of GT by atomic coordinates. However, it is not clear what technical effect could be associated with these claims. Thus, the underlying technical problem is the elucidation of the crystal structure of a GT. This is a scientific project, and not an invention characterised by a technical effect. Since there is no technical problem defined, said claims cannot be inventive.

Moreover, D2 describes the purification of the identical enzyme of the present application. D1 discloses the crystal structure of the GT, SpsA, from B. subtilis.

D3 provides extensive analytical data on sequences and structure comparisons by sequence alignments of over 500 GT. The obtention of crystals and X-ray structures from a member of theses GT families is a trivial problem.
As stated under point 2., claim 21 lacks a technical problem, and therefore an inventive step.
Claims 22-26 do not contain any special technical feature (see also point 2.).
Molecular modelling of protein ligands (e.g. inhibitors, substrates) and structure-based molecular design are well known in the prior art (e.g., D4 and D5). Thus, said claims are trivial.
The features of the present claims 28 and 30-33 are either trivial or conventional in the art or within the competence of a skilled man seeking to improve the prior art processes mentioned in the search report and in the present opinion.
Thus, all claims mentioned under this point are not inventive.

4. For the assessment of the present claims 31-33 on the question whether they are industrially applicable, no unified criteria exist in the PCT Contracting States. The patentability can also be dependent upon the formulation of the claims. The EPO, for example, does not recognize as industrially applicable the subject-matter of claims to the use of a compound in medical treatment, but may allow, however, claims to a known compound for first use in medical treatment and the use of such a compound for the manufacture of a medicament for a new medical treatment.

PATENT COOPERATION TREATY

PCT

INTERNATIONAL SEARCH REPORT

(PCT Article 18 and Rules 43 and 44)

Applicant's or agent's file reference	**FOR FURTHER ACTION** see Notification of Transmittal of International Search Report (Form PCT/ISA/220) as well as, where applicable, item 5 below.	
P174-PCT11		
International application No.	International filing date *(day/month/year)*	(Earliest) Priority Date *(day/month/year)*
PCT/CA 00/ 00725	16/06/2000	18/06/1999
Applicant		
RINI, James		

This International Search Report has been prepared by this International Searching Authority and is transmitted to the applicant according to Article 18. A copy is being transmitted to the International Bureau.

This International Search Report consists of a total of 5 sheets.

[X] It is also accompanied by a copy of each prior art document cited in this report.

1. **Basis of the report**

   a. With regard to the **language**, the international search was carried out on the basis of the international application in the language in which it was filed, unless otherwise indicated under this item.

   [ ] the international search was carried out on the basis of a translation of the international application furnished to this Authority (Rule 23.1(b)).

   b. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application, the international search was carried out on the basis of the sequence listing :

   [X] contained in the international application in written form.

   [ ] filed together with the international application in computer readable form.

   [ ] furnished subsequently to this Authority in written form.

   [X] furnished subsequently to this Authority in computer readble form.

   [X] the statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.

   [X] the statement that the information recorded in computer readable form is identical to the written sequence listing has been furnished

2. [X] **Certain claims were found unsearchable** (See Box I).

3. [ ] **Unity of invention is lacking** (see Box II).

4. With regard to the **title,**

   [X] the text is approved as submitted by the applicant.

   [ ] the text has been established by this Authority to read as follows:

5. With regard to the **abstract,**

   [X] the text is approved as submitted by the applicant.

   [ ] the text has been established, according to Rule 38 2(b). by this Authority as it appears in Box III. The applicant may, within one month from the date of mailing of this international search report, submit comments to this Authority.

6. The figure of the **drawings** to be published with the abstract is Figure No. _____

   [ ] as suggested by the applicant.

   [ ] because the applicant failed to suggest a figure

   [ ] because this figure better characterizes the invention.

   [X] None of the figures.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Although claim 31 is directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound/composition.

Although claims 34 and 35 could be considered as a mere presentation of information, Rule 39.1 (v and vi) PCT, the search has been carried out as far as possible in our systematic documentation

Continuation of Box I.2

Present claims 20 27 29 -32 relate to compounds defined by reference to a desirable characteristic or property, namely modulating glycosyltransferases
The claims cover all compounds having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for only UDP-GlcNAc. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the compound by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, the search has been carried out for those parts of the claims which appear to be clear, supported and disclosed, namely those parts relating to the UDP-GlcNAc.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

International Application No
PCT/EP 00/00725

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12N9/10 C12Q1/48 A61K31/70

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
BIOSIS, EPO-Internal

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	CHARNOCK SIMON J ET AL: "Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms." BIOCHEMISTRY, vol. 38, no. 20, 18 May 1999 (1999-05-18), pages 6380-6385, XP002152151 ISSN: 0006-2960	1-3,14, 15,20, 21,27, 29,34,35
Y	the whole document	18,19, 22-26, 28,30-32

-/--

[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
8 November 2000	22/11/2000

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	VAN DER SCHAAL, C

2

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
X	NISHIKAWA Y ET AL: "CONTROL OF GLYCOPROTEIN SYNTHESIS PURIFICATION AND CHARACTERIZATION OF RABBIT LIVER UDP-N-ACETYLGLUCOSAMINE ALPHA-3-D-MANNOSIDE BETA-1 2-N ACETYLGLUCOSAMINYLTRANSFERASE I" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 263, no. 17, 1988, pages 8270-8281, XP002152152 ISSN: 0021-9258	1-17,20, 21,27, 29,34,35
Y	the whole document	18,19, 22-26, 28,30-32
X	ULLMAN C AND PERKINS S: "A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities" BIOCHEMICAL JOURNAL, vol. 326, 1997, pages 929-941, XP002152153 page 937, paragraph 1	1-17,20, 21,27, 29,34,35
Y	DATABASE BIOSIS 'Online! BIOSCIENCES INFORMATION SERVICE, PHILADELPHIA, PA, US; 1994 SARKAR MOHAN: "Expression of recombinant rabbit UDP-GlcNAc:alpha-3-D-mannoside beta-1,2-N-acetylglucosaminyltransferase I catalytic domain in Sf9 insect cells." Database accession no. PREV199598004969 XP002152154 abstract & GLYCOCONJUGATE JOURNAL, vol. 11, no. 3, 1994, pages 204-209, ISSN: 0282-0080	18,19
Y	KUNTZ I D ET AL: "STRUCTURE-BASED MOLECULAR DESIGN" ACCOUNTS OF CHEMICAL RESEARCH,US,AMERICAN CHEMICAL SOCIETY. WASHINGTON, vol. 27, no. 5, May 1994 (1994-05), pages 117-123, XP000885741 ISSN: 0001-4842 cited in the application the whole document	20, 22-26, 28,30-33
Y	GSCHWEND D A ET AL: "MOLECULAR DOCKING TOWARDS DRUG DISCOVERY" JOURNAL OF MOLECULAR RECOGNITION,GB,HEYDEN & SON LTD., LONDON, vol. 9, 1996, pages 175-186, XP000882526 ISSN: 0952-3499 the whole document	20, 22-26, 28,30-33

2

PATENT COOPERATION TREATY

PCT

INTERNATIONAL SEARCH REPORT

(PCT Article 18 and Rules 43 and 44)

Applicant's or agent's file reference	**FOR FURTHER ACTION**	see Notification of Transmittal of International Search Report (Form PCT/ISA/220) as well as, where applicable, item 5 below.
P174-PCT11		
International application No.	International filing date *(day/month/year)*	(Earliest) Priority Date *(day/month/year)*
PCT/CA 00/ 00725	16/06/2000	18/06/1999
Applicant		
RINI, James		

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3. [ ] **Unity of invention is lacking** (see Box II).

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6. The figure of the **drawings** to be published with the abstract is Figure No. _____

   [ ] as suggested by the applicant.

   [ ] because the applicant failed to suggest a figure.

   [ ] because this figure better characterizes the invention.

   [X] None of the figures.

INTERNATIONAL SEARCH REPORT

[redacted] tional Application No
[redacted] CA 00/00725

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12N9/10 C12Q1/48 A61K31/70

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
BIOSIS, EPO-Internal

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
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Y	the whole document	18,19, 22-26, 28,30-32

	-/--	

[X] Further documents are listed in the continuation of box C. [ ] Patent family members are listed in annex.

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"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
8 November 2000	22/11/2000

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	VAN DER SCHAAL, C

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
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X	ULLMAN C AND PERKINS S: "A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities" BIOCHEMICAL JOURNAL, vol. 326, 1997, pages 929-941, XP002152153 page 937, paragraph 1	1-17,20, 21,27, 29,34,35

Y	DATABASE BIOSIS 'Online! BIOSCIENCES INFORMATION SERVICE, PHILADELPHIA, PA, US; 1994 SARKAR MOHAN: "Expression of recombinant rabbit UDP-GlcNAc:alpha-3-D-mannoside beta-1,2-N-acetylglucosaminyltransferase I catalytic domain in Sf9 insect cells." Database accession no. PREV199598004969 XP002152154 abstract & GLYCOCONJUGATE JOURNAL, vol. 11, no. 3, 1994, pages 204-209, ISSN: 0282-0080	18,19

Y	KUNTZ I D ET AL: "STRUCTURE-BASED MOLECULAR DESIGN" ACCOUNTS OF CHEMICAL RESEARCH,US,AMERICAN CHEMICAL SOCIETY. WASHINGTON, vol. 27, no. 5, May 1994 (1994-05), pages 117-123, XP000885741 ISSN: 0001-4842 cited in the application the whole document	20, 22-26, 28,30-33

Y	GSCHWEND D A ET AL: "MOLECULAR DOCKING TOWARDS DRUG DISCOVERY" JOURNAL OF MOLECULAR RECOGNITION,GB,HEYDEN & SON LTD., LONDON, vol. 9, 1996, pages 175-186, XP000882526 ISSN: 0952-3499 the whole document	20, 22-26, 28,30-33

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Although claim 31 is directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound/composition.

Although claims 34 and 35 could be considered as a mere presentation of information, Rule 39.1 (v and vi) PCT, the search has been carried out as far as possible in our systematic documentation

Continuation of Box I.2

Present claims 20 27 29 -32 relate to compounds defined by reference to a desirable characteristic or property, namely modulating glycosyltransferases
The claims cover all compounds having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for only UDP-GlcNAc. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the compound by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, the search has been carried out for those parts of the claims which appear to be clear, supported and disclosed, namely those parts relating to the UDP-GlcNAc.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

rnational application No.
PCT/CA 00/00725

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

see FURTHER INFORMATION sheet PCT/ISA/210

2. [X] Claims Nos.:
because they relate to parts of the International Application that dc not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:

see FURTHER INFORMATION sheet PCT/ISA/210

3. [ ] Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2. [ ] As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

4. [ ] No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

[ ] The additional search fees were accompanied by the applicant's protest.

[ ] No protest accompanied the payment of additional search fees.

PATENT COOPERATION TREATY

PCT

REC'D 04 OCT 2001
WIPO PCT

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

(PCT Article 36 and Rule 70)

Applicant's or agent's file reference	FOR FURTHER ACTION	See Notification of Transmittal of International Preliminary Examination Report (Form PCT/IPEA/416)
P174-PCT11		
International application No.	International filing date *(day/month/year)*	Priority date *(day/month/year)*
PCT/CA00/00725	16/06/2000	18/06/1999
International Patent Classification (IPC) or national classification and IPC C12N9/10		
Applicant RINI, James et al.		

1. This international preliminary examination report has been prepared by this International Preliminary Examining Authority and is transmitted to the applicant according to Article 36.

2. This REPORT consists of a total of 7 sheets, including this cover sheet.

   ☐ This report is also accompanied by ANNEXES, i.e. sheets of the description, claims and/or drawings which have been amended and are the basis for this report and/or sheets containing rectifications made before this Authority (see Rule 70.16 and Section 607 of the Administrative Instructions under the PCT).

   These annexes consist of a total of sheets.

3. This report contains indications relating to the following items:

   - I ☒ Basis of the report
   - II ☐ Priority
   - III ☒ Non-establishment of opinion with regard to novelty, inventive step and industrial applicability
   - IV ☐ Lack of unity of invention
   - V ☒ Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations suporting such statement
   - VI ☐ Certain documents cited
   - VII ☐ Certain defects in the international application
   - VIII ☒ Certain observations on the international application

Date of submission of the demand	Date of completion of this report
18/01/2001	02.10.2001
Name and mailing address of the international preliminary examining authority: European Patent Office D-80298 Munich Tel. +49 89 2399 - 0 Tx: 523656 epmu d Fax: +49 89 2399 - 4465	Authorized officer Strobel, A Telephone No. +49 89 2399 7362

Form PCT/IPEA/409 (cover sheet) (January 1994)

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/CA00/00725

I. Basis of the report

1. With regard to the **elements** of the international application *(Replacement sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred to in this report as "originally filed" and are not annexed to this report since they do not contain amendments (Rules 70.16 and 70.17))*:
Description, pages:

1-245 as originally filed

Claims, No.:

1-35 as originally filed

Drawings, sheets:

1/53-53/53 as originally filed

Sequence listing part of the description, pages:

1, as originally filed

2. With regard to the **language**, all the elements marked above were available or furnished to this Authority in the language in which the international application was filed, unless otherwise indicated under this item.

These elements were available or furnished to this Authority in the following language: , which is:

- ☐ the language of a translation furnished for the purposes of the international search (under Rule 23.1(b)).
- ☐ the language of publication of the international application (under Rule 48.3(b)).
- ☐ the language of a translation furnished for the purposes of international preliminary examination (under Rule 55.2 and/or 55.3).

3. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application, the international preliminary examination was carried out on the basis of the sequence listing:

- ☒ contained in the international application in written form.
- ☐ filed together with the international application in computer readable form.
- ☐ furnished subsequently to this Authority in written form.
- ☒ furnished subsequently to this Authority in computer readable form.
- ☒ The statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.
- ☒ The statement that the information recorded in computer readable form is identical to the written sequence listing has been furnished.

4. The amendments have resulted in the cancellation of:

- ☐ the description, pages:
- ☐ the claims, Nos.:
- ☐ the drawings, sheets:

5. ☐ This report has been established as if (some of) the amendments had not been made, since they have been considered to go beyond the disclosure as filed (Rule 70.2(c)):

   (Any replacement sheet containing such amendments must be referred to under item 1 and annexed to this report.)

6. Additional observations, if necessary:

III. Non-establishment of opinion with regard to novelty, inventive step and industrial applicability

1. The questions whether the claimed invention appears to be novel, to involve an inventive step (to be non-obvious), or to be industrially applicable have not been examined in respect of:

   ☐ the entire international application.

   ☒ claims Nos. 20, 27, 29-32 all partially, 34, 35 completely.

because:

   ☒ the said international application, or the said claims Nos. 34 and 35 relate to the following subject matter which does not require an international preliminary examination (*specify*):
   see separate sheet

   ☐ the description, claims or drawings (*indicate particular elements below*) or said claims Nos. are so unclear that no meaningful opinion could be formed (*specify*):

   ☐ the claims, or said claims Nos. are so inadequately supported by the description that no meaningful opinion could be formed.

   ☒ no international search report has been established for the said claims Nos. 20, 27, 29-32 all partially.

2. A meaningful international preliminary examination cannot be carried out due to the failure of the nucleotide and/or amino acid sequence listing to comply with the standard provided for in Annex C of the Administrative Instructions:

   ☐ the written form has not been furnished or does not comply with the standard.

   ☐ the computer readable form has not been furnished or does not comply with the standard.

V. Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)	Yes:	Claims	
	No:	Claims	1-7, 11, 13-16, 18-20, 27, 29
Inventive step (IS)	Yes:	Claims	
	No:	Claims	1-33
Industrial applicability (IA)	Yes:	Claims	1-30
	No:	Claims	

2. Citations and explanations
see separate sheet

VIII. Certain observations on the international application

The following observations on the clarity of the claims, description, and drawings or on the question whether the claims are fully supported by the description, are made:
see separate sheet

For reasons of better comprehension, the present opinion does not stick to the usual division into points I.-VIII.

Claims 1-10 and 14-19 are directed to two- or three-dimensional structures. The claims are therefore not directed to the product per se but only to the strucural information of the product. These claims are neither product claims nor method claims but appear to be mere presentation of information. The subject-matter of these claims is therefore, in principle, excluded from examination under Article 34(4)(a)(1) in combination with Rule 67.1(v) PCT.

Nevertheless, the following comments on novelty, inventive step, and clarity have been made:

Reference is made to the following documents:

D1: CHARNOCK SIMON J ET AL: 'Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms.' BIOCHEMISTRY, vol. 38, no. 20, 18 May 1999 (1999-05-18), pages 6380-6385

D2: NISHIKAWA Y ET AL: 'CONTROL OF GLYCOPROTEIN SYNTHESIS PURIFICATION AND CHARACTERIZATION OF RABBIT LIVER UDP-N-ACETYLGLUCOSAMINE ALPHA-3-D-MANNOSIDE BETA-1 2-N ACETYLGLUCOSAMINYLTRANSFERASE I' JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 263, no. 17, 1988, pages 8270-8281

D3: ULLMAN C AND PERKINS S: 'A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities' BIOCHEMICAL JOURNAL, vol. 326, 1997, pages 929-941

D4: KUNTZ I D ET AL: "STRUCTURE-BASED MOLECULAR DESIGN" ACCOUNTS OF CHEMICAL RESEARCH,US,AMERICAN CHEMICAL SOCIETY. WASHINGTON, vol. 27, no. 5, May 1994 (1994-05), pages 117-123

D5: GSCHWEND D A ET AL: "MOLECULAR DOCKING TOWARDS DRUG DISCOVERY" JOURNAL OF MOLECULAR RECOGNITION,GB,HEYDEN & SON LTD., LONDON, vol. 9, 1996, pages 175-186

1. Claims 20, 27, 29-32 have only been searched partially. Claims or parts of claims that have only been searched partially need not be the subject of an international preliminary examination, Rule 66.1(e) PCT. Thus, said claims are only examined with respect to UDP-GlcNAc.

Claims 34 and 35 concern the mere presentation of information and are thus

excluded from examination according to Rule 67.1(v) PCT.

2. **Clarity and Novelty**

Claims 1-7, 11, 13-16, and 18-33 do not fulfil the requirements of Article 6 PCT. The reasons for this lack of clarity are as follows:

Product claims 1-7, 11, 13-16, 18 and 19 directed to structures of glycosyltransferases (GT) do not define said structures at all or in a way that permits the man skilled in the art to clearly comprehend the subject-matter claimed. Said claims are so broad that they also are not novel over D1-3 which describe glycosyltransferases in solution or in crystal form as well as bound to substrates (Non-fulfilment of Article 33(2) PCT).

All claims directed to modulators, inhibitors of GT or methods for obtaining such modulators or inhibitors, namely claims 20, 22-33 are not supported by the description since, apart from the natural substrate UDP-GlcNAc, neither such compounds are disclosed nor are methods indicated that allow for the obtention of such compounds (i.e. the applicants actually do not provide any experimental data. If on the other hand the general and vague description of the claimed methods is sufficient for the obtention of such a compound, then said methods and compounds would certainly not be inventive). Of course, this objections holds also for the medical use of such hypothetical modulators, as defined in claims 31-33.

Claim 21 in its broadness lacks a recognisable technical problem and is therefor unclear.

Product claims have to be novel as such. D2 describes UDP-GlcNAc as a ligand of GTn-1. Thus, claims 20, 27, and 29 lack novelty (Article 33(2) PCT).

3. **Inventive step of claims 8-10, 12, 17, 21-26, 28, and 30-33**

Claims 8-10, 12 and 17 define structures of GT by atomic coordinates. However, it is not clear what technical effect could be associated with these claims. Thus, the underlying technical problem is the elucidation of the crystal structure of a GT. This is a scientific project, and not an invention characterised by a technical effect. Since there is no technical problem defined, said claims cannot be inventive.

Moreover, D2 describes the purification of the identical enzyme of the present application. D1 discloses the crystal structure of the GT, SpsA, from B. subtilis.

D3 provides extensive analytical data on sequences and structure comparisons by sequence alignments of over 500 GT. The obtention of crystals and X-ray structures from a member of theses GT families is a trivial problem.
As stated under point 2., claim 21 lacks a technical problem, and therefore an inventive step.
Claims 22-26 do not contain any special technical feature (see also point 2.).
Molecular modelling of protein ligands (e.g. inhibitors, substrates) and structure-based molecular design are well known in the prior art (e.g., D4 and D5). Thus, said claims are trivial.
The features of the present claims 28 and 30-33 are either trivial or conventional in the art or within the competence of a skilled man seeking to improve the prior art processes mentioned in the search report and in the present opinion.
Thus, all claims mentioned under this point are not inventive.

4. For the assessment of the present claims 31-33 on the question whether they are industrially applicable, no unified criteria exist in the PCT Contracting States. The patentability can also be dependent upon the formulation of the claims. The EPO, for example, does not recognize as industrially applicable the subject-matter of claims to the use of a compound in medical treatment, but may allow, however, claims to a known compound for first use in medical treatment and the use of such a compound for the manufacture of a medicament for a new medical treatment.

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(54) Title: GLYCOSYLTRANSFERASES STRUCTURES

(57) Abstract: The invention relates to the three dimensional structure of a glycosyltransferase. The atomic coordinates that define the structure and any compounds bound to the structure enable the determination of the three dimensional structures of glycosyltransferases with unknown structure, and the identification of modulators of a glycosyltransferase.

TITLE: Glycosyltransferases Structures

FIELD OF THE INVENTION

The invention relates to the secondary and three dimensional structures of glycosyltransferases. The atomic coordinates that define the structure and any compounds bound to the structure may be used to determine glycosyltransferase homologues and the structures of polypeptides with unknown structure, and to identify modulators of glycosyltransferases.

BACKGROUND OF THE INVENTION

The oligosaccharide chains of N- and O-linked glycoproteins play a crucial role in a number of biological processes. Their biosynthesis and degradation pathways are therefore areas of significant interest for biology, medicine, and biotechnology. The assembly of the various types of oligosaccharides involves several glycosidases and glycosyltransferases. In comparison with glycosidases, the mechanisms of which have been characterized in some detail, mechanistic investigations on glycosyltransferases have not yet undergone much scrutiny, although some kinetic studies have been reported.

Glycosyltransferases are a diverse group of enzymes that catalyze the transfer of a single monosaccharide unit from a donor to the hydroxyl group of an acceptor saccharide. The acceptor can be either a free saccharide, glycoprotein, glycolipid, or polysaccharide. The donor can be a nucleotide–sugar, or dolichol-phosphate-sugar. Glycosyltransferases show a precise specificity for both the sugar acceptor and donor, and generally require the presence of a metal cofactor.

SUMMARY OF THE INVENTION

Broadly stated, the present invention relates to the secondary and three-dimensional structures of glycosyltransferases, and parts thereof. The glycosyltransferase structure may be the structure the enzyme takes up when it is associated with one or more moieties (e.g. an acceptor, a sugar nucleotide donor, or components thereof). The invention also contemplates a glycosyltransferase structure comprising a secondary or three-dimensional structure of a glycosyltransferase in association with a moiety. The defined boundaries and properties of the structures and any of the moieties bound to it are pertinent to methods for determining the secondary or three-dimensional structures of polypeptides with unknown structure, and to methods that identify modulators of glycosyltransferases. These modulators are potentially useful as therapeutics for diseases, including (but not limited to) tumor growth, metastasis of tumors, bacterial, viral, and parasitic infections, and inflammatory diseases such as rheumatoid arthritis, asthma, inflammatory bowel disease, and atherosclerosis.

In an embodiment, the invention provides a crystalline form of a polypeptide corresponding to a glycosyltransferase, or a part thereof. The invention preferably contemplates a crystalline form a glycosyltransferase takes up when it is complexed with a moiety, including a nucleotide sugar donor, acceptor, metal cofactor, or heavy metal atom. The crystalline form may also comprise one or more heavy metal atoms, or at least one compound. A unit cell of the crystalline form of the invention may have dimensions of about a = 40.4 ± 3.0 Å, b=82.4 ± 3.0 Å, c = 102.5 ± 3.0 Å.

A glycosyltransferase structure of the invention may also be characterized by one or more of the following:

(a) an N-terminal domain (amino acid residues 106-317 in Table 3) comprising an eight-stranded mixed β-sheet (β1-β8 in Figure 25) flanked by six helices (α1-α6 in Figure 25) and a small two-stranded antiparallel β-sheet (β4' and β8' in Figure 25); and

(b) a C-terminal domain (amino acid residues 354-447 in Table 3) comprising a four-stranded mixed β-sheet (β9, β10, β13, and β14 in Figure 25) flanked by three α-helices (α7-α9 in Figure 25) and a short β-finger (β11 and β12 in Figure 25).

The N-terminal domain and C-terminal domain may be connected by a linker region (residues 331 to 353 in Table 3) which wraps halfway around the N-terminal domain before starting the first helix of the C-terminal domain.

The crystalline form may also be specifically characterized by the parameters, diffraction statistics and/or refinement statistics set out in Table 6.

The invention also contemplates a secondary or three-dimensional structure (e.g. a crystalline form) of a domain of a glycosyltransferase. In accordance with one aspect, the invention contemplates a secondary or three-dimensional structure of a domain comprising an eight-stranded mixed β-sheet, flanked by six helices and a small two-stranded antiparallel β-sheet. The domain is also referred to herein as the "spsA GnT 1 core domain" or "SGC domain". In accordance with a preferred embodiment, the invention contemplates a domain comprising an eight-stranded mixed β-sheet represented as β1-β8 in Figure 25, flanked by six helices represented by α1-α6 in Figure 25, and a small two-stranded antiparallel β-sheet represented by β4' and β8' in Figure 25. A secondary or three-dimensional structure of a polypeptide comprising an SGC domain of the invention is also within the scope of the invention.

The invention further contemplates a loop structure of a glycosyltransferase. A loop structure may be characterized as the structure adjacent to the nucleotide-sugar donor binding site comprising amino acid residues 318-330 in Table 3. The loop structure may be further characterized by amino acid residues 320-323 forming a type IV turn and amino acid residues 324-330 making one complete turn of an α-helix. A secondary or three dimensional structure of a polypeptide comprising a loop structure of the invention is also within the scope of the invention.

The invention also relates to a method of forming a crystalline form of the invention.

The invention also features a method of determining secondary or three-dimensional structures of polypeptides with unknown structure comprising the step of applying the structural atomic coordinates of a crystalline form of a glycosyltransferase of the invention.

The invention also provides a secondary or three-dimensional structure of a binding site of a glycosyltransferase. Binding sites include the binding sites for one or more of a disphosphate or pyrophosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, a sugar of the nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, and/or an acceptor. The secondary or three-dimensional structure of a binding site may be defined by selected atomic contacts in the site. Thus, broadly stated the present invention provides a secondary or three-dimensional structure of a binding site of a glycosyltransferase defined by one or more atomic interactions or enzyme

atomic contacts as set forth in Table 5. Each of the atomic interactions is defined in Table 5 by an atomic contact (more preferably, a specific atom where indicated) on the sugar nucleotide donor or acceptor, and an atomic contact (more preferably a specific atom where indicated) on the glycosyltransferase.

The invention also relates to modulators derived from a secondary or three-dimensional structure of a glycosyltransferase, binding sites, atomic interactions, or atomic contacts thereof, or a domain of a secondary or three-dimensional structure of a glycosyltransferase, including a SGC domain. Preferably, the modulators are derived from binding sites for a sugar nucleotide donor or parts thereof, an acceptor or parts thereof, including the SGC domain, and the binding site described herein as the loop structure. The invention provides inhibitors that are derived from a DxD motif, for example, peptides having the sequences as shown in Figures 27 and 31 (SEQ ID NOs 1-9).

The present invention also contemplates a method of identifying a modulator of a glycosyltransferase, a binding site or a domain thereof, comprising the step of using the structural coordinates of a glycosyltransferase, binding sites, atomic interactions, or atomic contacts thereof, or domain thereof, to computationally evaluate a test compound for its ability to associate with the glycosyltransferase, binding site, or domain thereof. Use of the structural coordinates of a glycosyltransferase structure, binding sites, atomic interactions, or atomic contacts of the invention to identify a modulator is also provided.

In an embodiment of the invention, a method is provided for identifying a modulator of a glycosyltransferase by determining binding interactions between a test compound and a binding site of a glycosyltransferase, or atomic interactions, or atomic contacts thereof, or a domain of a glycosyltransferase defined in accordance with the invention comprising:

(a) generating the binding site, atomic interactions, atomic contacts, or domain on a computer screen;

(b) generating a test compound with its spatial structure on the computer screen; and

(c) testing to determine whether the test compound binds to the binding site, a selected number of atomic contacts, or the domain.

Methods are also provided for identifying a potential modulator of a glycosyltransferase function by docking a computer representation of a compound with a computer representation of a structure of a glycosyltransferase or a part thereof, that is defined by the atomic structural coordinates, atomic interactions, or atomic contacts described herein.

In an embodiment the method comprises the following steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of a selected site (e.g. the sugar nucleotide donor or acceptor binding site, loop structure, or SGC domain) on a glycosyltransferase defined in accordance with the invention, to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying compounds that best fit the selected site as potential modulators of the glycosyltransferase.

In another embodiment the method comprises the following steps:

(a) modifying a computer representation of a compound complexed with a selected site (e.g. sugar nucleotide donor or acceptor binding site, loop structure, or SGC domain) on a glycosyltransferase defined in accordance with the invention, by deleting or adding a chemical group or groups;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying a compound that best fits the selected site as a potential modulator of a glycosyltransferase.

In still another embodiment the method comprises the following steps:

(a) selecting a computer representation of a compound complexed with a selected site (e.g. sugar nucleotide donor or acceptor binding site, loop structure, or SGC domain) on a glycosyltransferase defined in accordance with the invention; and

(b) searching for molecules in a data base that are similar to the compound using a searching computer program, or replacing portions of the compound with similar chemical structures from a data base using a compound building computer program.

A compound that interacts with a glycosyltransferase, binding sites or atomic contacts thereof, or a domain thereof, identified using a method of the invention may be used as a modulator of any glycosyltransferase or composition bearing the interacting binding site, atomic contacts, or domain. Therefore, the invention features a modulator of a glycosyltransferase identified by a method of the invention.

The invention further contemplates classes of modulators of glycosyltransferases based on the three-dimensional structure of a sugar nucleotide donor, or component thereof, or acceptor, defined in relation to the sugar nucleotide donor's or acceptor's spatial association with a glycosyltransferase structure. Generally, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of a sugar nucleotide donor or acceptor or component thereof, defined in relation to it spatial association with the glycosyltransferase structure or a binding site thereof, to generate a compound that is capable of associating with the glycosyltransferase or binding site thereof.

It will be appreciated that a modulator of a glycosyltransferase may be identified by generating an actual secondary or three-dimensional models of a binding site, synthesizing a compound, and examining the components to find whether the required interaction occurs.

A potential modulator of a glycosyltransferase identified by a method of the present invention may be confirmed as a modulator by synthesizing the compound, and testing its effect on the glycosyltransferase in an assay for that glycosyltransferase's enzymatic activity. Such assays are known in the art.

A modulator of the invention may be converted using customary methods into pharmaceutical compositions. A modulator may be formulated into a pharmaceutical composition containing a modulator either alone or together with other active substances.

Therefore, the methods of the invention for identifying modulators may comprise one or more of the following additional steps:

(a) testing whether the modulator is a modulator of the activity of a glycosyltransferase, preferably testing the activity of the modulator in cellular assays and animal model assays;

(b) modifying the modulator;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

Steps (a), (b) (c) and (d) may be carried out in any order, at different points in time, and they need not be sequential.

The invention also contemplates a method of treating a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism, comprising:

(a) administering a modulator of the invention in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting a glycosyltransferase to treat the disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism. Use of the structural coordinates of a glycosyltransferase structure of the invention to manufacture a medicament is also provided.

Another aspect of the invention provides machine readable media encoded with data representing the coordinates of the secondary or three dimensional structure of a glycosyltransferase, binding sites or atomic contacts thereof, or domain as defined herein, or the three dimensional structure of a sugar nucleotide donor or acceptor defined in relation to its spatial association with a glycosyltransferase structure as defined herein. The invention also provides computerized representations of the secondary or three-dimensional structures of the invention, including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation.

These and other aspects of the present invention will become evident upon reference to the following detailed description and attached drawings.

DESCRIPTION OF THE DRAWINGS

The invention will now be described in relation to the drawings in which:

Figure 1 is a secondary structure diagram of GnT-1, as viewed along the beta sheet, from strand "b3." Note the eight-stranded beta sheet twist in the foreground, and the four-stranded beta sheet, offset in the background.

Figure 2 is a secondary structure diagram of GnT-1, showing a view from the side. The first domain is a mixed eight-stranded beta sheet, backed by alpha helices, indicated by "b" for the beta strands and "a" for the alpha helices. The second domain is a mixed four-stranded beta sheet, again backed by helices, and indicated with capital "B" and "A," respectively.

Figure 3 is a sample of experimental MAD MeHg-derivative GnT-1 density, from the bottom of the active site pocket. The Hg position was identified using SOLVE. SHARP was used to refine the Hg parameters, and CCP4 dm was used for solvent-flattening and histogram matching, giving the shown map.

Figure 4 is a hydrophobic surface diagram of the top and bottom of GnT-1, with hydrophobic regions in green. Note the patch in the pocket, as well as at the base of the alpha-helix "tower."

Figure 5 is an electrostatic surface diagram of the top and bottom of GnT-1, with acidic regions in red, and basic regions in blue. Note the large acidic patch to one side of the active site pocket.

Figure 6 is a conservation diagram of the active site pocket of GnT-1. Conserved regions are indicated in red, with "A" being fully conserved, and "0" unconserved. Alignments of active GnT-1's (rabbit, human, rat, mouse, golden hamster, chinese hamster, *C. elegans* 1 #1 and #3, and frog) was performed using CLUSTALX, and conservation was calculated using AMAS. Note the highly conserved active site pocket.

Figure 7 is a worm diagram of the GnT-I structure with secondary structure shown. Beta strands are shown as arrows, and alpha helices are helices. UDP-GlcNAc and the Mn^{2+} ion are shown in the binding site.

Figure 8A through 8F are surface diagrams of the GnT-I structure.UDP-GlcNAc and the Mn^{2+} ion are shown in the binding site. (8A) The phosphate-binding loop lid, which forms upon UDP-GlcNAc binding, is shown as a worm. (8B) The loop is shown as a surface. (8C) The surface has been colored according to potential. Basic potential is shown in blue, and acidic potential is shown in red; the loop is shown as a worm. (8D) As in 8C, but with the loop shown as a surface. (8E) The surface has been colored according to residue AMAS conservation index. Red regions are conserved, white are unconserved; the loop is shown as a worm. (8F) As in 8E, but with the loop shown as a surface.

Figure 9 are diagrams showing the active site of the GnT-1 enzyme. Asp291 is shown as a stick figure on the left side of the pocket, while the rest of the protein is shown as a surface. UDP-GlcNAc is shown as a stick figure on the right. Mn^{2+} has been shown as a sphere. (9A) The loop is shown as a worm. (9B) The loop is shown as a surface. Note the mannose-sized active site pocket.

Figure 10 is a surface diagram of GnT-1 bound to the model of the $Man_5GlcNAc_2$ acceptor. UDP-GlcNAc is shown as a stick, and the Mn^{2+} has been shown as a sphere. (10A) The acceptor model is shown as a stick figure. (10B) The acceptor has been shown as a space-filling van der Waals figure.

Figure 11 is the same as Figure 10 but from a different angle, showing the fit of the acceptor to the surface more visible. (11A) The acceptor has been shown as a stick figure, and the loop as a worm. (11B) The acceptor has been shown as a stick figure, and the loop as a surface. (11C) The acceptor has been shown as space-filling van der Waals spheres, and the loop as a surface. (11D) As in 11B, but with the surface colored according to residue conservation index. Note the correlation of the acceptor model to red conserved residues.

Figure 12 shows a model of the active site of GnT-1, with the base D291 (i.e. Asp292), the α-1,3 mannose O2, and the GlcNAc C1 joined by lines of small spheres. The protein backbone has been shown as an alpha-carbon trace, the acceptor $Man_5GlcNAc_2$ sugar, UDP-GlcNAc, and protein side-chains have been shown as stick figures, and the Mn^{2+} ion and bound water molecules have been shown as spheres.

Figure 13 shows a model of the overlay of GnT-1 (red), *Bacillus subtilis* nucleotide- diphospho-sugar transferase (spsA) (green), *Escherichia coli* N-acetylglucosamine 1-phosphate uridyltransferase (GlmU) (blue), and bovine β-1,4-galactosyltransferase T1 (galT) (cyan). Parts of the protein sequence not in the transferase fold are shaded a darker color.

Figure 14 shows the overlay of GnT-1 and GlmU from the model of Figure 13. The DALI z-score (a measure of structural similarity) for this overlay is 9.6. Dissimilar structures give scores less than 2; greater similarity gives a higher score.

Figure 15 shows the overlay of GnT-1 and β-1,4-galT from the model of Figure 13. The DALI z-score for this overlay is 10.6.

Figure 16 shows the overlay of GnT-1 and spsA from the model of Figure 13. The DALI z-score for this overlay is 15.7.

Figure 17 shows the model of Figure 13 from a different angle. Note the overlay of the helix-loop-helix containing the catalytic base Asp residue (Asp 291 in GnT-1, Asp 191 in spsA, and Asp in galT).

Figure 18 shows the overlay of GnT-1 and GlmU from the model of Figure 17.

Figure 19 shows the overlay of GnT-1 and galT from the model of Figure 17.

Figure 20 shows the overlay of GnT-1 and spsA from the model of Figure 17.

Figure 21 shows the secondary structure of GnT-1. Helices are in red and β sheets are in green. Areas not in the conserved fold are darkened.

Figure 22 shows the secondary structure of GlmU. Helices are in red and β sheets are in green. β strand 6 has been deleted.

Figure 23 shows the secondary structure of galT. Helices are in red and β sheets are in green. β strand 3 has been deleted along with helix 2 leading into it. Instead, a small β finger N-terminal of the core domain and a β finger C-terminal of the core domain occupy the space of β strand 3.

Figure 24 shows the secondary structure of spsA. Helices are in red and β sheets are in green. All eight strands are present in the core domain.

Figure 25 is a GnT I Ribbon Diagram. Domain 1 is shown in cyan, the loop (residues 318 to 330) structured upon UDP-GlcNAc binding in red, the linker connecting Domain 1 and Domain 2 in green, Domain 2 in brown, and the UDP-GlcNAc and the Mn^{2+} ion are shown in yellow. All molecular images were prepared using SPOCK (Christopher, 1998) and rendered using Raster3D (Bacon, 1988 ; Merritt, 1994).

Figure 26 shows the electrostatic potential surface of GnT I, showing the acidic pocket into which the Mn^{2+} ion and UDP-GlcNAc bind. Acidic residues are colored red, and basic residues blue, with a gradient through ±10 kT. The UDP-GlcNAc is shown in yellow.

Figure 27 shows a sample of the AMAS analysis. Shown is an excerpt from the AMAS analysis, with residues in the region of the "DxD" motif (residues 211 to 213, EDD). GnT I sequences from rabbit human, mouse, rat, Chinese hamster, golden hamster, frog, and *C.elegans* genes gly-12 and gly-14, were aligned using ClustalX, and conservation was scored using AMAS. Unconserved residues are given a score of "0", and fully conserved residues are given a score of "A". (SEQ ID NO 1, 2, 3, 4, and 5).

Figure 28 shows AMAS surface analysis. AMAS residue scores, as shown in Figure 27, were then mapped onto the protein surface, with a gradient from green for a completely unconserved score of 0, to white for an AMAS score of 5, to red for a fully conserved score of "A".

Figure 29 shows a stereo ribbon overlay of the SGC domains of GnT 1 (red) and spsA (green). For clarity only the α-helices are labeled. UDP (spsA) and UDP-GlcNAc (GnT1) are shown in stick representation. M and C label the side chains of the metal binding and catalytic aspartic acid residues also shown in stick representation

Figure 30 shows topology diagrams of GnT I, spsA, GlmU (an N-acetylglucosamine-1 -phosphate

uridyltransferase from *Escherichia coli*) and β4Gal-T1 (a bovine galactosyl transferase, β-1,4-galactosyltransferase 1). Beta strands are shown as green triangles, and alpha helices as red circles, with missing elements shown in white. The secondary structural elements are labeled as in GnT I. The boxed gray region corresponds to the SGC domain..

Figure 31 shows a structural alignment of GnT I, spsA, GlmU and β4Gal-T1. (SEQ ID NO 6, 7, 8, and 9). Shown are two excerpts from the complete alignment, numbered according to rabbit GnT I. In the top alignment, the region around the DxD motif is shown, with the motif highlighted in magenta. In the bottom alignment, the area around the catalytic Asp is shown, with the catalytic residue again highlighted in magenta. Note that GlmU is not a glycosyltransferase, but rather an N-acetylglucosamine-1-phosphate uridyl transferase, so it does not share the catalytic residue found in GnT I, spsA, and β4Gal-T1 .

Figure 32 shows the GnT I substrate binding site. All interactions between the protein, the UDP-GlcNAc, the Mn^{2+} ion, and structured waters are shown as lines composed of small white spheres.

Figure 33A, B, and C show a stereo view of the UDP-GlcNAc/Mn^{2+} binding site. Carbon, oxygen, nitrogen, sulfur, and phosphorus are colored white, red, blue, yellow and purple respectively; water molecules are cyan and the Mn^{2+} ion is salmon. Hydrogen bonds are shown as dotted lines. The C1 of the *N*-acetylglucosamine moiety is labeled for reference. 33A Uracil and ribose interactions; 33B) Mn^{2+} and phosphate interactions; 33C) *N*-acetylglucosamine interactions.

Figure 34 shows interactions between GnT I, the Mn^{2+} ion, and the UDP-GlcNAc phosphates. R117 is from the N-terminus of helix α1, E211 and D213 are from the C-terminus of strand β4, T315 and G317 are from strand β8' and the N-terminus of the loop lid, and V321 and S322 are from the tip of the loop lid.

Figure 35 shows interactions between GnT I and the GlcNAc group of UDP-GlcNAc. Residue Y184 is in helix α3, residue E211 is in strand β4, residue L269 is from the C-terminus of strand β7, residues F289, W290, D291 and R295 are from helix α6, and L331 is from the C-terminal end of the loop lid. D291 is the only Asp that is close enough to the GlcNAc C1 to act as the catalytic base.

Figure 36 shows GnT I overlaid on spsA: GnT I appears in red, and spsA in green. In this Figure, the position of the ligands is shown. GnT I is bound to UDP-GlcNAc, shown as a red stick figure, along with a Mn^{2+} ion, shown as a red sphere near Asp213; spsA is bound to UDP, shown as a green stick figure, along with a Mn^{2+} ion, shown as a green sphere near Asp 99. Note how the nucleotides and proteins overlay very closely. The catalytic base residue in GnT I, Asp 291, identified by this structure, has an analogous residue in spsA, Asp 191. This predicts that Asp 191 is the catalytic base in spsA. The catalytic base was not identifiable with the spsA x-ray crystal structure alone, due to the absence in the spsA structure of the sugar residue normally attached to the UDP.

Figure 37 shows GnT I overlaid on β1, 4-galT: GnT I appears in red, and β-1,4-galT in cyan. Again, the ligands of GnT I are shown, as in Figure 36. The ligand in the β-1,4-galT x-ray crystal structure, UDP, is shown as a stick figure; the Mn^{2}+ normally required in the reaction is absent, as is the sugar part of the donor sugar-nucleotide. Again, GnT I's Asp 291 has an analogous galT residue, Asp318. This predicted to be the catalytic base in β-1,4-galT by the GnT I structure.

Figure 38 shows GnT I overlaid on GlmU: GnT I appears in red, and GlmU in navy blue. The ligands

of GnT I are shown in red, as in Figures 36 and 37. The GlmU product, UDP-GlcNAc, is shown as a navy blue stick figure. As GlmU is not a transferase, these two enzymes do not catalyse the same reaction, and thus the residues involved in enzymatic action are expected to be different. However, the similar fold and similar location of sugar-nucleotide binding, suggests that these enzymes may have evolved from an extremely distant common ancestor.

Figure 39 shows the DxD Motif. Atom colors and labels are as in Figure 33. Letters i, to i+3 correspond to the residues of the type 1 β-turn. The hydrogen bond characteristic of this turn type is shown in green.

Figure 40A and 40B shows a stereo diagram of the structured loop and the acceptor binding pocket. Atom colors and labels as in Figure 33. Backbone tubes and molecular surfaces are color coded as follows: red, structured loop; green, linker region; cyan, Domain 1; brown, Domain 2. 40A) Structured loop and UDP-GlcNAc/Mn^{2+} interactions; 40B) Surface representation of the acceptor binding pocket. The side chain of the catalytic base (D291) and the *N*-acetylglucosamine moiety of the UDP-GlcNAc are seen at the base of the pocket.

DETAILED DESCRIPTION OF THE INVENTION

Summary of Tables 1 to 8

Table 1- structural coordinates of an N-acetylglucosaminyl transferase I (GnT-1) native structure.

Table 2 –structural coordinates of a GnT-1 with bound MeHg .

Table 3 –structural coordinates of a rabbit GnT-1 bound to UDP-GlcNAc and a manganese 2+ ion.

Table 4 – structural coordinates of a GnT-1 with acceptor.

Table 5 – Intermolecular Contacts of GnT-1-UDP-GlcNAc Complex.

Table 6 - crystallographic data and refinement statistics.

Table 7 - The UDP-GlcNAc binding site.

Table 8 – Protein threading results.

In Tables 1 to 4, from the left, the second column identifies the atom number; the third identifies the atom type; the fourth identifies the amino acid type; the fifth identifies the residue number; the sixth identifies the x coordinates; the seventh identifies the y coordinates; the eighth identifies the z coordinates; the ninth identifies the occupancy; and the eleventh identifies the temperature factor.

Definitions:

Unless otherwise indicated, all terms used herein have the same meaning as they would to one skilled in the art of the present invention. Practitioners are particularly directed to Current Protocols in Molecular Biology (Ansubel) for definitions and terms of the art.

"Glycosyltransferase structure" or "glycosyltransferase secondary or three-dimensional structure" refers to the three-dimensional structure (i.e. tertiary structure) or arrangement of secondary structural elements of a purified polypeptide comprising a glycosyltransferase. A glycosyltransferase structure may be in association with or complexed with a moiety including a heavy metal atom or metal cofactor. A glycosyltransferase structure may be in crystalline form.

The term "crystalline form" in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide comprising a glycosyltransferase. The glycosyltransferase is , preferably a glycosyltransferse with an SGC domain, including but not limited to a glycosyltransferase structurally related to N-acetylglucosaminyltransferase I to VIII, preferably N-acetylglucosaminyltransferase I. A crystalline form of a glycosyltransferase, is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al 1976, Protein Crystallography, Academic Press. A crystalline form may include a crystal structure in association with one or more moieties, including heavy-metal atoms i.e. a derivative crystal, or one or more compounds i.e. a co-crystal.

The term "associate", "association" or "associating" refers to a condition of proximity between a moiety (i.e. chemical entity or compound or portions or fragments thereof), and a glycosyltransferase, or parts or fragments thereof (e.g. binding sites or domains). The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy-metal atoms" refers to an atom that can be used to solve an x-ray crystallography phase problem, including but not limited to a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

A "metal cofactor" refers to a metal ion required for a glycosyltransferase to transfer the selected sugar from the sugar nucleotide donor to the acceptor. For example, the metal cofactor for N-acetylglycosyltransferase may be a divalent cation like manganese, or magnesium, and other similar atoms or metals.

The term "glycosyltransferase" refers to an enzyme that catalyzes the transfer of a single monosaccharide unit from a donor to the hydroxyl group of an acceptor substrate. The acceptor can be either a free saccharide, glycoprotein, glycolipid, or polysaccharide. The donor can be a nucleotide–sugar, or dolichol-phosphate–sugar. Glycosyltransferases show a precise specificity for both the sugar acceptor and donor and generally require the presence of a metal cofactor. The term "glycosyltransferase" also encompasses polypeptides comprising a SGC domain.

Glycosyltransferases include but are not limited to eukaryotic glycosyltransferases involved in the biosynthesis of glycoproteins, glycolipids, glycosylphosphatidylinositols and other complex glycoconjugates, and prokaryotic glycosyltransferases involved in the synthesis of carbohydrate structures of bacteria and viruses, including enzymes involved in LOS and lipopolysaccharide biosynthesis. Examples of glycosyltransferases include N-acetylglucosaminyltransferases, including N-acetylglucosaminyltransferases I through VIII involved in the biosynthesis of complex and hybrid N-glycans; UDP-N-acetylglucosamine:N-acetyl galactosamine β1,6-N-acetylglucosaminyl transferases (core 2 GlcNAc transferases); Core 3 GlcNAc transferase, Core 4 GlcNAc transferase; Core1 and Core 2 elongation glycosyltransferases involved in the biosynthesis of O-glycans and the glycosyltransferases involved in the biosynthesis of antigen determinants (blood group i and blood group I); and structurally related proteins.

The enzyme at the gateway from high-mannose structures to hybrid and complex *N*-glycans is UDP-

N-acetylglucosamine:α-3-D-mannoside β-1,2-*N*-acetylglucosaminyltransferase I [GnT I; E.C. 2.4.1.101; Harpaz and Schachter, 1980; Narasimhan et al, 1977; Stanley et al, 1975; See GenBank M61829 and M55621 (human) and M57301 (rabbit) for nucleic acid and amino acid sequences]. It transfers the first *N*-acetylglucosamine residue onto the high-mannose core and all other enzymes in the hybrid and complex pathway depend on its prior action (Schachter, 1986; Schachter, 1991). GnT I plays a fundamental role in mammalian development, as shown by knockout studies in mice (Ioffe, 1994; Metzler, 1994). Moreover, mutation or misregulation of several of the enzymes dependent on GnT I action are associated with human disease and metastasis (Jaeken et al, 1994,; Charuk et al, 1995; Jaeken et al , 1993; Granovsky et al, 2000; Tan et al, 1996).

Glycosyltransferases have been classified into 44 different families, based on both sequence similarity and substrate/product stereochemistry (inverting or retaining) (Campbell et al, 1997; Campbell et al, 1998; Coutinho and Henrissat, 1999). GnT I (family 13) is an inverting glycosyltransferase: the α-linked GlcNAc moiety from the UDP-α-GlcNAc donor is transferred to the 3-arm of the $Man_5GlcNAc_2$ acceptor, creating the β-linked GlcNAc-β-1,2-Man-R product (Reck et al, 1994).

As applied to polypeptides, the term "substantial sequence identity" means that two peptide sequences, when optimally aligned, such as by the programs GAP or BESTFIT using default gap, share at least 40%, 50%, 60%, 65%, 70%, 75%, 80%, or 85% sequence identity, preferably at least 90 percent sequence identity, more preferably at least 95 percent sequence identity or more. Preferably, residue positions which are not identical differ by conservative amino acid substitutions. For example, the substitution of amino acids having similar chemical properties such as charge or polarity are not likely to effect the properties of a protein. Examples include glutamine for asparagine or glutamic acid for aspartic acid.

The term "mutant" refers to a polypeptide that is obtained by replacing at least one amino acid residue in a native glycosyltransferase with a different amino acid residue. Mutation can also be accomplished by adding and/or deleting amino acid residues within the native glycosyltransferase or part thereof. A mutant may or may not be functional.

The term "function" refers to the ability of a modulator to enhance or inhibit the association between a glycosyltransferase and a compound, or the activity of the glycosyltransferase.

"Modulator" refers to a molecule which changes or alters the biological activity of a glycosyltransferase. A modulator may increase or decrease glycosyltransferase activity, or change its characteristics, or functional or immunological properties. It may be an inhibitor that decreases the biological or immunological activity of the protein. Modulators include but are not limited to peptides, members of random peptide libraries and combinatorial chemistry-derived molecular libraries, phosphopeptides (including members of random or partially degenerate, directed phosphopeptide libraries), antibodies, carbohydrates, nucleosides or nucleotides or parts thereof, and small organic or inorganic molecules. A modulator may be an endogenous physiological compound, or it may be a natural or synthetic compound.

The term "atomic structural coordinates" or "structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules (e.g. Cartesian coordinates, temperature factors, and occupancies). Structural coordinates can be slightly modified and still render nearly identical three

dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures (in particular a three dimensional structure of an SGC domain) that deviate from one another by a root-mean-square deviation of less than 5 Å, 4 Å, 3 Å, 2 Å, or 1.5 Å may be viewed by a person of ordinary skill in the art as very similar.

The term "unit cell" refers to the smallest and simplest volume element (i.e. parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The unit cell axial lengths are represented by a, b, and c. Those of skill in the art understand that a set of atomic coordinates determined by X-ray crystallography is not without standard error.

The term "space group" refers to the lattice and symmetry of the crystal. In a space group designation the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the contents of the asymmetric unit without changing its appearance.

The term "purified" in reference to a polypeptide, does not require absolute purity such as a homogenous preparation rather it represents an indication that the polypeptide is relatively purer than in the natural environment. Generally, a purified polypeptide is substantially free of other proteins, lipids, carbohydrates, or other materials with which it is naturally associated, preferably at a functionally significant level for example at least 85% pure, more preferably at least 95% pure, most preferably at least 99% pure. A skilled artisan can purify a polypeptide comprising a glycosyltransferase using standard techniques for protein purification. A substantially pure polypeptide comprising a glycosyltransferase will yield a single major band on a non-reducing polyacrylamide gel. The purity of the glycosyltransferase can also be determined by amino-terminal amino acid sequence analysis.

A "sugar nucleotide donor" refers to a nucleotide coupled to a selected sugar that is transferred by a glycosyltransferase to an acceptor. The selected sugar may be a monosaccharide. A suitable selected sugar includes N-acetyl glucosamine (GlcNAc). The N-acetyl glucosamine may be modified for example, the hydroxyls may be blocked with acetonide, acylated, or alkylated or substituted with other groups such as halogen. For N-acetylglucosaminyltransferases the nucleotide is preferably UDP. For other enzymes, the nucleotide may be GDP (fucosyltransferases and mannosyltransferases), or CMP (sialyltransferases). The heterocyclic amine base in the nucleotide may be modified. For example, when the base is uridine it may be modified at the C-5 or C-6 position with groups including but not limited to alkyl, aryl, and electron donating and electron withdrawing groups. The sugar in the nucleotide (e.g. ribose) may be modified at the 2' or 3' position with groups including but not limited to alkyl, aryl, and electron donating and electron withdrawing groups.

"Acceptor" refers to the part of a carbohydrate structure (e.g. glycoprotein, glycolipid) where the selected sugar is transferred by the glycosyltransferase. The acceptor may comprise $Man_5GlcNAc_2$-.

Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids.

Glycosyltransferase Structures

The present invention provides a secondary or three-dimensional structure of a glycosyltransferase or part thereof (e.g. binding site or domain). In an embodiment the structure is a crystalline form. A

glycosyltransferase structure may comprise a glycosyltransferase in a unit cell. In an embodiment, a glycosyltransferase is arranged in a crystallline manner in a space group $P2_12_12_1$ so as to form a unit cell of dimensions a= 40.4 ± 3.0 Å, b= 82.4 ± 3.0 Å, c= 102.5 ± 3.0 Å, $\alpha=\beta=\gamma= 90°$, and which effectively diffracts X-rays for determination of the atomic coordinates of a glycosyltransferase. The secondary and three-dimensional structure of a preferred glycosyltransferase of the invention is illustrated by the N-acetyl glucosaminyl transferase I (GnT 1) structure specifically described herein. A glycosyltransferase structure may be defined by the structural coordinates of Tables 1, 2, 3, or 4.

A glycosyltransferase structure includes the secondary or three-dimensional structure of a native glycosyltransferase, a derivative glycosyltransferse, or a mutant glycosyltransferase. Thus, a crystalline form includes native crystals, derivative crystals, and co-crystals. The crystals generally comprise a substantially pure glycosyltransferase in crystalline form. It is understood that the glycosyltransferase structures of the invention are not limited to a naturally occurring or native glycosyltransferases but include polypeptides comprising an SGC domain, or polypeptides with substantial sequence identity to a glycosyltransferase. A glycosyltransferase structure also includes mutants of a native glycosyltransferase obtained by replacing at least one amino acid residue in a native glycosyltransferase with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide, and having substantially the same secondary or three-dimensional structure as the native glycosyltransferase from which the mutant is derived i.e. having a set of atomic structural coordinates that have a root mean square deviation of less than or equal to about 5, 4, 3, 2, or 1.5 Å when superimposed with the atomic structure coordinates of the native glycosyltransferase from which the mutant is derived when at least 50% to 100% of the atoms of the native glycosyltransferase domain are included in the superimposition. It should be noted that the glycosyltransferase structures contemplated herein need not exhibit glycosyltransferase activity.

A derivative glycosyltransferase structure of the invention comprises a glycosyltransferase structure in association with one or more moieties that are heavy metal atoms. For example, derivative crystals of the invention generally comprise a crystalline glycosyltransferase in covalent association with one or more heavy metal atoms. The glycosyltransferase may correspond to a native or mutated glycosyltransferase. Heavy metal atoms useful for providing derivative glycosyltransferase structures include by way of example, and not limitation, gold, mercury, etc.

The invention features a glycosyltransferase structure in association with one or more moieties that are compounds (e.g. UDP-GlcNAc, uridine-ribose, phosphate-Mn^{2+}, $Man_5GlcNAc_2$-, one or more metal cofactors). The association may be covalent or non-covalent. Crystalline forms of this type are referred to herein as co-crystals. The compound may be any organic molecule, and it may modulate the function of a glycosyltransferase by for example inhibiting or enhancing its function, or it may be an acceptor, donor, or metal cofactor for the glycosyltransferase. It is preferred that the geometry of the compound and the interactions formed between the compound and the glycosyltransferase provide high affinity binding between the two molecules.

The secondary or three-dimensional structures of the particular glycosyltransferases described herein provide useful models for the secondary or three-dimensional structures of glycosyltransferases from any

species, particularly mammalian, including bovine, ovine, porcine, murine, equine, preferably human, from any source whether natural, synthetic, semi-synthetic, or recombinant.

Binding Sites - The GnT-1 active site

N-acetylglucosaminyltransferase I catalyses the addition of a β-1,2 GlcNAc onto the α-1,3 arm of the $Man_5GlcNAc_2$ N-linked carbohydrate moiety. The structure has allowed the identification of the binding site of UDP-GlcNAc, identification of the reaction centre, and the development of a working model of the $Man_5GlcNAc_2$-acceptor binding site that correlates with biochemical reaction inhibition evidence.

The UDP-GlcNAc binding site can be subdivided into three sub sites: the uridine-ribose binding sub site, the phosphate-Mn^{2+} binding sub site, and the GlcNAc sub site.

In the uridine-ribose sub site, there are three direct hydrogen bonds between the protein and the nucleotide sugar. Asp144 interacts with the uridine N3, the His190 ND1 interacts with the uridine O2, and Asp212 binds the ribose O3. In addition, there is one water-mediated bond between Asp212 and the ribose O2. Meanwhile, the uridine base makes van der Waals interactions with Ile187, as well as the cysteine bridge between Cys115 and Cys145.

The phosphate-Mn^{2+} site is the subject of many interactions between the nucleotide sugar and protein; in fact, while the manganese co-ordination site lies on the enzyme's surface, a majority of the interactions with the phosphates come from a loop which structures itself on top of the substrate upon binding.

The protein itself has only one direct co-ordination bond to the Mn^{2+}, via Asp213; since two of the six co-ordination points are taken up by the phosphate oxygens (one from each phosphate), the final three points are bound by water. These waters are then bound by the Thr315 OG, the Gly317 carbonyl oxygen, Glu211 and Asp213.

The phosphate groups make one direct hydrogen bond to Arg317NH on the protein's rigid surface, while making three hydrogen bonds with the flexible loop which rigidifies into a lid on top of the phosphate-Mn^{2+} subsite. These loop interactions are with the Val321 backbone N and the backbone N and OG of Ser322. In addition, a two-water hydrogen-bonding bridge leads to Asp116.

In contrast to the previous two sub sites, which hold the UDP-GlcNAc rigidly in place, the GlcNAc-binding sub site must allow the sugar ring enough flexibility to go through the flat penta-coordinate C1 intermediate. Three direct hydrogen bonds are made: two between the GlcNAc O4 and Asp211 and Trp290, anchoring the O4-C1 axis of the GlcNAc in place, and one between the GlcNAc O3 and Asp211, establishing the correct pucker for the sugar ring. One water bridge also exists between the sugar and the protein; the GlcNAc O6 hydrogen bonds to a water molecule held in place by the amide nitrogens of Phe289 and Trp290, along with the carbonyl oxygen of Tyr184.

The acetyl group methyl makes van der Waals contact with Leu269 and Leu331, leaving the acetyl group O7 and N2, along with the GlcNAc ring O5, unbonded. This lack of interaction may give the C2 and O5 enough flexibility to make the movements necessary for the C1 to achieve the reaction intermediate sn2 conformation.

This experimental nucleotide-sugar binding conformation has allowed the identification of the base in the reaction: Asp291 is located just over 5 Å from the GlcNAc C1, putting it in a perfect position to perform this role.

The identification of the reaction centre and binding site has provided the constraints necessary to make a theoretical model of the $Man_5GlcNAc_2$-acceptor binding site. The α-1,3 mannose O2 is placed between the Asp291 OD1 and the GlcNAc C1, putting it into position for the nucleophilic attack on the C1. This positioning forces the conformation of the rest of the mannose: the O3 forms hydrogen bonds to Asp291, Arg295, and a structured water held in place by Arg415; the O4 hydrogen bonds to the same structured water as the O3; and the O6 hydrogen bonds to both a UDP-GlcNAc phosphate, as well as the OG of Ser322, a phosphate-binding lid loop residue. This α-1,3 mannose orientation corresponds with biochemical evidence that all of the mannose ring's hydroxyl groups are important. In addition, this model supports the ordered-sequential reaction sequence, as the GlcNAc is buried below the $Man_5GlcNAc_2$, as well as further evidence that the $Man_5GlcNAc_2$ binding site is partially formed upon GnT-1's UDP-GlcNAc binding.

The $Man_5GlcNAc_2$ core mannose position is also constrained by the reaction centre location: the O4 hydrogen bonds to asp291, the ring is in van der Waals contact with Phe289 and Tyr184, and the O6 hydrogen bonds to Asp292. Again, this position supports the known biochemistry, as the O4 is important, the O2 is unimportant, and the β O1 linkage is required to allow the ring to sit against the protein surface. An α O1 would clash with the protein, and may break up the important lectin-like van der Waals interaction with the phenylalanine.

Finally, the model allows the positioning of the α-1,6 mannose, the α-1,3 and α-1,6 mannoses attached to it, and the chitobiosyl-core $GlcNAc_2$. The positions of these sugar rings in the model correspond with the location of conserved GnT-1 surface residues; biochemical evidence states that these sugars are less important to $Man_5GlcNAc_2$ binding, and thus their position is less well defined than the α-1,3 arm and core mannose.

In summary, the *N*-acetylglucosaminyltransferase I structure has allowed the exact identification of the UDP-GlcNAc binding site, along with the reaction centre, and allowed the prediction of the $Man_5GlcNAc_2$-acceptor binding site. This UDP-GlcNAc-bound, closed-loop GnT-1 structure is critical for the design of high-affinity inhibitors to the activity of GnT-1.

Therefore, the invention contemplates a secondary or three-dimensional structure of a binding site of a glycosyltransferase. Binding sites include the binding site for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, a sugar of the nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, and/or an acceptor. A three dimensional structure of a binding site may be defined by selected atomic contacts, preferably the enzyme atomic contacts as defined in Table 5.

In an embodiment of the invention, a secondary or three-dimensional structure of a binding site of a glycosyltransferase that associates with a diphosphate of a sugar nucleotide donor (or the secondary or three-dimensional structure of a complex of the binding site with the diphosphate) is provided comprising at least

two or three atomic contacts of atomic interactions 8, 9, and 10 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the diphosphate group, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact). The binding site may be defined by the enzyme atomic contacts of atomic interactions 8 and 9; 8 and 10; 9 and 10; or 8, 9, and 10 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

In an embodiment of the invention, a secondary or three-dimensional structure of a binding site of a glycosyltransferase that associates with a heterocyclic amine base (preferably uracil) of a sugar nucleotide donor (or the secondary or three-dimensional structure of a complex of the binding site with a heterocyclic amine base) is provided comprising at least two, three, or four atomic contacts of atomic interactions 1, 2, 3, 4, and 5 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the heterocyclic amine base, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact).. The binding site may be defined by the enzyme atomic contacts of atomic interactions 1, 2, and 3; 2, 3, and 4; 3, 4, and 5; 1,2, and 4; 1,2, and 5; 1, 3, and 4; 1, 3, and 5; 2, 3, and 5; 2, 4, and 5; 1, 2, 3, and 4; 1,2, 3, and 5; 2, 3, 4, and 5; 1, 3, 4, and 5; or 1, 2, 3, 4, and 5 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

In an embodiment of the invention, a secondary or three-dimensional structure of a binding cavity of a glycosyltransferase that associates with the sugar of the nucleotide (preferably ribose) of a sugar nucleotide donor (or a secondary or three-dimensional structure of a complex of the binding site with the sugar) is provided comprising the atomic contacts of atomic interactions 6 and 7 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the sugar, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact). The binding site may be defined by the enzyme atomic contacts of atomic interactions 6 and 7 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts in the binding site having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

In an embodiment of the invention, a secondary or three-dimensional structure of a binding cavity of a glycosyltransferase that associates with a selected sugar (GlcNAc) of a sugar nucleotide donor (or a secondary or three-dimensional structure of a complex of the binding site with the selected sugar) is provided comprising at least two, three, four, five, six, seven, or eight atomic contacts selected from the atomic contacts of atomic interactions 14, 15, 16, 17, 18, 19, 20, and 21 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the selected sugar, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact).. The binding site may be defined by the enzyme atomic contacts of atomic interactions 14, 18, and 19; 14, 20, and 21; 14, 15, 16, and 17; 18, 19, 20, and 21; and 14 through 21 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts in the binding site having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

In an embodiment of the invention, a secondary- or three-dimensional structure of a binding cavity of a glycosyltransferase that associates with a nucleotide (preferably UDP) of a sugar nucleotide donor (or a secondary or three-dimensional structure of a complex of the binding site and nucleotide) is provided comprising at least two, three, four, five, six, seven, or eight, nine or ten atomic contacts of atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, and 10 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the nucleotide, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact). The binding site may be defined by enzyme atomic contacts of atomic interactions 1, 2, 6, 7, 8, 9, and 10; 3, 4, 6, 7, 8, 9, and 10; and 1 through 10 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts in the binding site having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

In an embodiment of the invention, a secondary- or three-dimensional structure of a binding cavity of a glycosyltransferase that associates with a sugar nucleotide donor (e.g. UDP-GlcNAc) (or a secondary or three-dimensional structure of a complex of the binding site with the sugar nucleotide donor) is provided comprising at least two, three, four, five, six, seven, eight, nine, ten, eleven, twelve, thirteen, fourteen, fifteen, sixteen, seventeen, eighteen, nineteen, twenty, or twenty-one atomic contacts of atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, and 21 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the sugar nucleotide donor, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact). The binding site may be defined by enzyme atomic contacts of atomic interactions 1,2, 6, 7, 8, 9, 10, 14, 15, 18, and 20; 1, 2, 6, 7, 8, 9, 10, 14, 16, 17, 19, and 21; 3, 4, 6, 7, 8, 9, 10, 14, 15, 18, and 20; 3, 4, 6, 7, 8, 9, 10, 14, 16, 17, 19, 21; or 1 through 21 listed in Table 5. Preferably the binding site is defined by the atoms of the enzyme atomic contacts in the binding site having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

A glycosyltransferase structure may be characterized by a "loop" structure. The loop folds on top of the pyrophosphate after the sugar nucleotide donor associates with the active site of the glycosyltransferase. Molecules that associate with the loop are highly specific inhibitors of the enzymes. In an embodiment of the invention, a secondary or three-dimensional structure of a loop structure of a glycosyltransferase that binds a pyrophosphate of a sugar nucleotide donor is provided comprising at least two, three, four, five, six, or seven atomic contacts of atomic interactions 11, 12, 13, 23, 24, 25, and 27 in Table 5. The binding site may be defined by enzyme atomic contacts 11, 12, and 13; 11, 12, 13 and 27; 23, 24, 25, and 27; or 11, 12, 13, 23, 24, 25, and 27 in Table 5.Preferably, the binding site is defined by the atoms of the enzyme atomic contacts in the binding site have the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

A secondary or three-dimensional structure of a binding site of a glycosyltransferase that associates with an $Man_5GlcNAc_2$-acceptor (or a secondary or three dimensional structure of a complex of the binding site with the acceptor) is also provided comprising at least two, three, four, five, or six atomic contacts of atomic interactions 22, 23, 24, 25, 26, and 27 in Table 5, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the acceptor, and an atomic contact (more preferably, a

specific amino acid residue where indicated) on the glycosyltransferase (i.e. enzyme atomic contact). The binding site may be defined by enzyme atomic contacts of atomic interactions 22, 23, and 24; 23, 24, and 25; 24, 25, and 26; 25, 26, and 27; 22, 23, 24, and 25; 23, 24, 25, and 26; 24, 25, 26, and 27; 22, 23, 24, 25, and 26; 23, 24, 25, 26, and 27; and 22 through 27 in Table 5. Preferably, the binding site is defined by the atoms of the enzyme atomic contacts in the binding site having the structural coordinates for the atoms listed in Table 1, 2, 3, or 4.

Method for Preparing Crystal Forms of a Glycosyltransferase

The invention also features a method for creating crystalline glycosyltransferase structures described herein. The method may utilize a polypeptide comprising a glycosyltransferase described herein to form a crystal. A polypeptide used in the method may be chemically synthesized in whole or in part using techniques that are well-known in the art. Alternatively, methods are well known to the skilled artisan to construct expression vectors containing the native or mutated glycosyltransferase coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination. See for example the techniques described in Sambrook et al. (Molecular Cloning: A Laboratory Manual, 2nd Edition, Cold Spring Harbor Laboratory press (1989)), and other laboratory textbooks. (See also Sarker et al, Glycoconjugate J. 7:380, 1990; Sarker et al, Proc. Natl. Acad, Sci. USA 88:234-238, 1991, Sarker et al, Glycoconjugate J. 11: 204-209, 1994; Hull et al, Biochem Biophys Res Commun 176:608, 1991 and Pownall et al, Genomics 12:699-704, 1992).

Crystals are grown from an aqueous solution containing the purified glycosyltransferase polypeptide by a variety of conventional processes. These processes include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. (See for example, McPherson, 1982 John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189: 1-23; Webber. 1991, Adv. Protein Chem. 41:1-36). Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the glycosyltransferase polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

In an embodiment of the invention, the method comprises mixing a volume of a glycosyltransferase solution (e.g. 5 mg glycosyltransferase /ml to 15 mg glycosyltransferase /ml, preferably 10 mg/ml) with a reservoir solution; and equilibrating against the reservoir solution under vapour-diffusion conditions.

It will be appreciated that the crystallization conditions can be varied and such variations can be used alone or in combination.

Derivative crystals of the invention can be obtained by soaking native crystals in a solution containing salts of heavy metal atoms. A complex of the invention can be obtained by soaking a native crystal in a solution containing a compound that binds the glycosyltransferase, or they can be obtained by co-crystallizing the glycosyltransferase polypeptide in the presence of one or more compounds that bind to the glycosyltransferase.

Once the crystal is grown it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those skilled in the art (See for example, Ducruix and Geige, 1992, IRL Press, Oxford, England). A beam of X-rays enter the crystal and diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Suitable devices include the Marr 345 imaging plate detector system with an RU200 rotating anode generator.

Methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and known to those skilled in the art (see Ducruix and Geige). Generally, the x-ray crystal structure is given by the diffraction patterns. Each diffraction pattern reflection is characterized as a vector and the data collected at this stage determines the amplitude of each vector. The phases of the vectors may be determined by the isomorphous replacement method where heavy atoms soaked into the crystal are used as reference points in the X-ray analysis (see for example, Otwinowski, 1991, Daresbury, United Kingdom, 80-86). The phases of the vectors may also be determined by molecular replacement (see for example, Naraza, 1994, Proteins 11:281-296). The amplitudes and phases of vectors from the crystalline form of a glycosyltransferase, e.g. an N-acetylglucosaminyltransferase I, determined in accordance with these methods can be used to analyze other crystalline glycosyltransferases, particularly those with an SGC domain.

The unit cell dimensions and symmetry, and vector amplitude and phase information can be used in a Fourier transform function to calculate the electron density in the unit cell i.e. to generate an experimental electron density map. This may be accomplished using the PHASES package (Furey, 1990). Amino acid sequence structures are fit to the experimental electron density map (i.e. model building) using computer programs (e.g. Jones, TA. et al, Acta Crystallogr A47, 100-119, 1991). This structure can also be used to calculate a theoretical electron density map. The theoretical and experimental electron density maps can be compared and the agreement between the maps can be described by a parameter referred to as R-factor. A high degree of overlap in the maps is represented by a low value R-factor. The R-factor can be minimized by using computer programs that refine the structure to achieve agreement between the theoretical and observed electron density map. For example, the XPLOR program, developed by Brunger (1992, Nature 355:472-475) can be used for model refinement.

A three dimensional structure of the molecule or complex may be described by atoms that fit the theoretical electron density characterized by a minimum R value. Files can be created for the structure that defines each atom by coordinates in three dimensions.

Identification of Homologues

The knowledge of a glycosyltransferase structure of the invention enables one skilled in the art to identify homologues of glycosyltransferases. This is achieved by searches of three-dimensional databases. Since structural folds are conserved to a greater extent than sequence, one may identify homologues with very little sequence identity or similarity. Programs that provide this type of database searching are known in the art and include Dali. The structural coordinates of a protein structure are submitted and the program performs a multiple structural alignment with proteins in the protein data bank. Homologues identified in accordance with the present invention may be used in the methods of the invention described herein.

Methods for Determining Secondary or Three Dimensional Structures

The structure coordinates of a glycosyltransferase structure described herein can be used as a model for determining the secondary or three-dimensional structures of additional native or mutated glycosyltransferases with unknown structure, as well as the structures of co-crystals of glycosyltransferases with compounds such as acceptors, donors (e.g. UDP-GlcNAc or analogues thereof), and modulators (e.g. stimulators or inhibitors). The structure coordinates and models of a glycosyltransferase structure can also be used to determine solution-based structures of native or mutant glycosyltransferases.

Secondary or three-dimensional structure may be determined by applying the structural coordinates of a glycosyltransferase structure to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (e.g. native or mutated glycosyltransferases). In the present invention the method utilizes a computer representation of a glycosyltransferase structure, preferably a three dimensional structure of an N-acetylglucosaminyltransferase I, or a complex of same, a computer representation of the amino acid sequence of a polypeptide with an unknown structure (additional native or mutated glycosyltransferases, or polypeptides comprising an SGC domain), and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating coordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art (Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, http://biochem.vt.edu/courses/modeling/homology.htn). Computer programs that can be used in homology modeling are Quanta and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modeling method, the known glycosyltransferase structure (e.g. structure of the N-acetylglucosaminyltransferase I) is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as alpha-helices and beta-sheets, and to ligand- and substrate-binding sites (e.g. acceptor and donor binding sites). The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch

[J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-10919, 1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used; however, other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modeled. A variety of approaches known to those skilled in the art may be used to assign coordinates to the unknown. In particular, the coordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain coordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

Molecular replacement involves applying a known structure to solve the X-ray crystallographic data set of a polypeptide of unknown structure (e.g. native or mutated glycosyltransferases). The method can be used to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. Commonly used computer software packages for molecular replacement are X-PLOR (Brunger 1992, Nature 355: 472-475), AMoRE (Navaza, 1994, Acta Crystallogr. A50:157-163), the CCP4 package (Collaborative Computational Project, Number 4, "The CCP4 Suite: Programs for Protein Crystallography", Acta Cryst., Vol. D50, pp. 760-763, 1994), and the MERLOT package (P.M.D. Fitzgerald,

J. Appl. Cryst., Vol. 21, pp. 273-278, 1988). It is preferable that the resulting structure not exhibit a root-mean-square deviation of more than 3 Å.

Molecular replacement computer programs generally involve the following steps: (1) determining the number of molecules in the unit cell and defining the angles between them (self rotation function); (2) rotating the known structure (e.g. glycosyltransferase) against diffraction data to define the orientation of the molecules in the unit cell (rotation function); (3) translating the known structure in three dimensions to correctly position the molecules in the unit cell (translation function); (4) determining the phases of the X-ray diffraction data and calculating an R-factor calculated from the reference data set and from the new data wherein an R-factor between 30-50% indicates that the orientations of the atoms in the unit cell have been reasonably determined by the method; and (5) optionally, decreasing the R-factor to about 20% by refining the new electron density map using iterative refinement techniques known to those skilled in the art (refinement).

In an embodiment of the invention, a method is provided for determining three dimensional structures of polypeptides with unknown structure (e.g. additional native or mutated glycosyltransferases) by applying the structural coordinates of a glycosyltransferase structure to provide an X-ray crystallographic data set for a polypeptide of unknown structure, and (b) determining a low energy conformation of the resulting structure.

The structural coordinates of a glycosyltransferase structure may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides (e.g. additional native or mutated glycosyltransferases, or polypeptides comprising an SGC domain). (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide defined by X-ray crystallography can guide the NMR spectroscopist to an understanding of the spatial interactions between secondary structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

In an embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, preferably a native or mutated glycosyltransferases or polypeptides comprising an SGC domain, by applying the structural coordinates of a glycosyltransferase structure of the invention to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term " through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

Identification of Modulators of Glycosyltransferases

Modulators (e.g. inhibitors) of a glycosyltransferase (or a binding site or domain thereof) may be designed and identified that may modify the inappropriate activity of a glycosyltransferase involved in a clinical disorder. The rational design and identification of modulators of glycosyltransferases can be accomplished by utilizing the atomic structural coordinates that define a glycosyltransferase structure, or a part thereof. Structure-based modulator design identification methods are powerful techniques that can involve searches of computer data bases containing a variety of potential modulators and chemical functional groups. (See Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; and Colman, 1994, Current Opinion in Struc. Biol. 4: 868, for reviews of structure-based drug design and identification;and Kuntz et al 1982, J. Mol. Biol. 162:269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623 for methods of structure-based modulator design).

The glycosyltransferase structures, and parts thereof described herein, and the structures of other polypeptides determined by the homology modeling, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods.

Modulators of glycosyltransferases may be identified by docking the computer representation of compounds from a data base of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

The computer programs may comprise the following steps:

(a) docking a computer representation of a structure of a compound into a computer representation of an active-site (e.g. binding site or SGC domain) of a glycosyltransferase defined in accordance with the invention using the computer program, or by interactively moving the representation of the compound into the representation of the active-site;

(b) characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compound; optionally

(c) searching libraries for molecular fragments which can fit into the empty space between the compound and active site and can be linked to the compound; and

(d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

Methods are also provided for identifying a potential modulator of a glycosyltransferase function by docking a computer representation of a compound with a computer representation of a structure of a glycosyltransferase that is defined by the binding sites, atomic interactions, atomic contacts, or atomic structural coordinates described herein. In an embodiment the method comprises the following steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of a selected site (e.g. the sugar nucleotide donor or acceptor binding site, or SGC domain) on a glycosyltransferase structure defined in accordance with the invention to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying compounds that best fit the selected site as potential modulators of the glycosyltransferase.

"Docking" refers to a process of placing a compound in close proximity with an active site of a polypeptide (i.e. a glycosyltransferase), or a process of finding low energy conformations of a compound/polypeptide complex (i.e. compound/glycosyltransferase complex).

Examples of other computer programs that may be used for structure-based modulator design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, J. Comp. Aided Molec. Design 8:153); PRO Modulator (Clark et al., 1995 J. Comp. Aided Molec. Design 9:13); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Fuction, and Genetics 8:195); and, GRID (Goodford, 1985, J. Med. Chem. 28:849).

In an embodiment of the invention, a method is provided for identifying potential modulators of glycosyltransferase function. The method utilizes the structural coordinates of a glycosyltransferase three dimensional structure, or binding site or domain thereof. The method comprises the steps of (a) generating a computer representation of a glycosyltransferase structure, preferably an N-acetylglucosaminyltransferase I structure, and docking a computer representation of a compound from a computer data base with a computer representation of an active site (e.g. sugar nucleotide donor or acceptor binding site) of the glycosyltransferase to form a complex; (b) determining a conformation of the complex with a favourable geometric fit or favorable complementary interactions; and (c) identifying compounds that best fit the glycosyltransferase active-site as potential modulators of glycosyltransferase function. The initial glycosyltransferase structure may or may not have compounds bound to it. A favourable geometric fit occurs when the surface areas of a compound in a compound-glycosyltransferase complex is in close proximity with the surface area of the active-site of the glycosyltransferase without forming unfavorable interactions. A favourable complementary interaction occurs where a compound in a compound-glycosyltransferase complex interacts by hydrophobic, aromatic, ionic, or hydrogen donating and accepting forces, with the active-site of a glycosyltransferase without forming unfavorable interactions. Unfavourable interactions may be steric hindrance between atoms in the compound and atoms in the glycosyltransferase active-site.

In another embodiment, potential modulators are identified utilizing a glycosyltransferase structure with or without compounds bound to it. The method comprises the steps of (a) modifying a computer representation of a glycosyltransferase (e.g. an N-acetylglucosaminyltransferase I) having one or more compounds bound to it, where the computer representations of the compound or compounds and glycosyltransferase are defined by atomic structural coordinates; (b) determining a conformation of the

complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the glycosyltransferase active site as potential modulators. A computer representation may be modified by deleting or adding a chemical group or groups. Computer representations of the chemical groups can be selected from a computer database.

Another way of identifying potential modulators is to modify an existing modulator in a polypeptide active-site. The computer representation of modulators can be modified within the computer representation of a glycosyltransferase active-site. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI. The computer representation of a modulator may be modified by deleting a chemical group or groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and active-site can be shifted in conformation and the distance between the modulator and the active site atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. Compounds with favourable scores are potential modulators.

Compounds designed by modulator building or modulator searching computer programs may be screened to identify potential modulators. Examples of such computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates). A building program may be used to replace computer representations of chemical groups in a compound complexed with a glycosyltransferase with groups from a computer data base. A searching program may be used to search computer representations of compounds from a computer database that have similar three dimensional structures and similar chemical groups as a compound that binds to a glycosyltransferase. The programs may be operated on the structure of the active-site (e.g. binding sites, or SGC domain) of a glycosyltransferase structure, preferably an N-acetylglucosaminyltransferase I.

A typical program may comprise the following steps:

(a) mapping chemical features of a compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;

(b) adding geometric constraints to selected mapped features;

(c) searching data bases with the model generated in (b).

In an embodiment of the invention a method of identifying potential modulators of a glycosyltransferase, preferably an N-acetylglucosaminyltransferase I, is provided using the three dimensional conformation of the glycosyltransferase in various modulator construction or modulator searching computer programs on compounds complexed with the glycosyltransferase. The method comprises the steps of (a) generating a computer representation of one or more compounds complexed with a glycosyltransferase; (b) (i) searching a data base for a compound with a similar geometric structure or similar chemical groups to the generated compounds using a computer program that searches computer representations of compounds from a database that have similar three dimensional structures and similar chemical groups, or (ii) replacing portions of the compounds complexed with the glycosyltransferase with similar chemical structures (i.e. nearly identical shape and volume) from a database using a compound construction computer program that replaces computer

representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

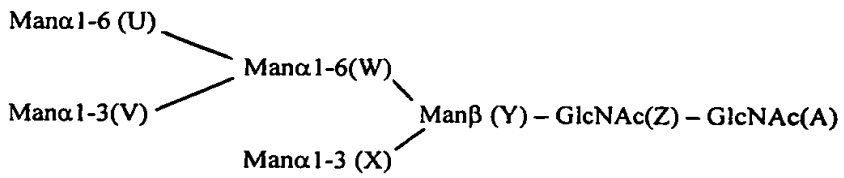
A compound that interacts with a glycosyltransferase or selected binding sites or domains thereof identified using a method of the invention may be used as a modulator of any glycosyltransferase or composition bearing the interacting binding site or domains. Therefore, the invention features a modulator of a glycosyltransferase identified by a method of the invention.

The invention further contemplates a method for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of a sugar nucleotide donor or acceptor or component thereof, or an acceptor or components thereof, defined in relation to its spatial association with a glycosyltransferase structure or a binding site or domain thereof, to generate a compound that is capable of associating with the glycosyltransferase or binding site or domain thereof.

In an embodiment of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of uridine, uracil, or UDP listed in Table 3 [ATOMS 2828-2835 (uracil); 2836-2844 (ribose); and 2845-2851 (diphosphate)] to generate a compound for associating with the active site of a glycosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of uridine, uracil, or UDP, defined by its structural coordinates listed in Table 3; (b) searching for molecules in a data base that are structurally or chemically similar to the defined uridine, uracil, or UDP, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

In another embodiment of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of UDP-GlcNAc listed in Table 3 (ATOMS 2813-2851), to generate a compound for associating with the active site of a glycosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of UDP-GlcNAc defined by its structural coordinates listed in Table 3; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined UDP-GlcNAc using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

In another embodiment of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of a $Man_5GlcNAc_2$ acceptor listed in Table 4, to generate a compound for associating with the active site of a glycosyltransferase. In Table 4, the coordinates of a $Man_5GlcNAc_2$ acceptor are listed as ATOMS 3043 through 3126 where the mannose and GlcNAc residues designated as X, Y, U, V, W, Z, and A have the following positions in the acceptor :



The following steps are employed in a particular method of the invention: (a) generating a computer representation of a $Man_5GlcNAc_2$ acceptor defined by its structural coordinates listed in Table 4; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined $Man_5GlcNAc_2$ acceptor using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

It will be appreciated that a modulator of a glycosyltransferase may be identified by generating an actual three-dimensional model of a binding cavity, synthesizing a compound, and examining the components to find whether the required interaction occurs.

Potential modulators of glycosyltransferases identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

The invention also relates to a potential modulator identified by the methods of the invention. In particular, classes of modulators of glycosyltransferases are provided that are based on the three-dimensional structure of a sugar nucleotide donor, or component thereof, or acceptor, defined in relation to the sugar nucleotide donor's or acceptor's spatial association with a glycosyltransferase structure. Modulators of glycosyltransferases comprise a compound comprising the structure of uracil, uridine, ribose, pyrophosphate, or UDP, and having one or more, preferably all, of the structural coordinates of uracil, uridine, ribose, pyrophosphate, or UDP of Table 3 [ATOMS 2828-2835 (uracil); 2836-2844 (ribose); and 2845-2851 (diphosphate)]. In an embodiment, modulators are provided comprising the structure of UDP-GlcNAc and having one or more, preferably all, of the structural coordinates of UDP-GlcNAc of Table 3 (ATOMS 2813-2851). Functional groups in the uracil, uridine, ribose, pyrophosphate, UDP, or UDP-GlcNAc modulators may be substituted with, for example, alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo, or they may be modified using techniques known in the art.

Modulators are also contemplated that comprise the structure of a $Man_5GlcNAc_2$ acceptor for a glycosyltransferase with the structural coordinates of $Man_5GlcNAc_2$ acceptor listed in Table 4 (ATOMS 3043 through 3126). Functional groups in an acceptor structure may be substituted with, for example, alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo, or they may be modified using techniques known in the art.

The invention contemplates all optical isomers and racemic forms of the modulators of the invention.

Compositions and Methods of Treatment

The modulators of the invention may be used to modulate the biological activity of a glycosyltransferase in a cell, including modulating a pathway in a cell regulated by the glycosyltransferase or modulating a glycosyltransferase with inappropriate activity in a cellular organism. In addition, a glycosyltransferase structure of the invention may be used to devise protocols to modulate the biological activity of a glycosyltransferase in a cell.

Cellular assays, as well as animal model assays *in vivo*, may be used to test the activity of a potential modulator of a glycosyltransferase as well as diagnose a disease associated with inappropriate

glycosyltransferase activity. *In vivo* assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

The modulators (e.g. inhibitors) identified using the methods of the invention may be useful in the treatment and prophylaxis of tumor growth and metastasis of tumors. Anti-metastatic effects of inhibitors can be demonstrated using a lung colonization assay. For example, melanoma cells treated with an inhibitor may be injected into mice and the ability of the melanoma cells to colonize the lungs of the mice may be examined by counting tumor nodules on the lungs after death. Suppression of tumor growth in mice by the inhibitor administered orally or intravenously may be examined by measuring tumor volume.

An inhibitor identified using the invention may have particular application in the prevention of tumor recurrence after surgery i.e. as an adjuvant therapy.

An inhibitor may be especially useful in the treatment of various forms of neoplasia such as leukemias, lymphomas, melanomas, adenomas, sarcomas, and carcinomas of solid tissues in patients. In particular, inhibitors can be used for treating malignant melanoma, pancreatic cancer, cervico-uterine cancer, ovarian cancer, cancer of the kidney such as metastatic renal cell carcinoma, stomach, lung, rectum, breast, bowel, gastric, liver, thyroid, head and neck cancers such as unresectable head and neck cancers, lymphangitis carcinamatosis, cancers of the cervix, breast, salivary gland, leg, tongue, lip, bile duct, pelvis, mediastinum, urethra, bronchogenic, bladder, esophagus and colon, non-small cell lung cancer, and Kaposi's Sarcoma which is a form of cancer associated with HIV-infected patients with Acquired Immune Deficiency Syndrome (AIDS). The inhibitors may also be used for other anti-proliferative conditions such as bacterial and viral infections, in particular AIDS.

An inhibitor identified in accordance with the present invention may be used to treat immunocompromised subjects. For example, they may be used in a subject infected with HIV, or other viruses or infectious agents including bacteria, fungi, and parasites, in a subject undergoing bone marrow transplants, and in subjects with chemical or tumor-induced immune suppression.

Inhibitors may be used as hemorestorative agents and in particular to stimulate bone marrow cell proliferation, in particular following chemotherapy or radiotherapy. The myeloproliferative activity of an inhibitor of the invention may be determined by injecting the inhibitor into mice, sacrificing the mice, removing bone marrow cells and measuring the ability of the inhibitor to stimulate bone marrow proliferation by directly counting bone marrow cells and by measuring clonogenic progenitor cells in methylcellulose assays. The inhibitors can also be used as chemoprotectants, and in particular to protect mucosal epithelium following chemotherapy.

An inhibitor identified in accordance with the invention also may be used as an antiviral agent in particular on membrane enveloped viruses such as retroviruses, influenza viruses, cytomegaloviruses and herpes viruses. An inhibitor may also be used to treat bacterial, fungal, and parasitic infections. For example, a small molecule inhibitor can be used to prevent or treat infections caused by the following: *Neisseria* species such as *Neisseria meningitidis*, and *N. gonorrheae*; *Chlamydia* species such as *Chlamydia pneumoniae*, *Chlamydia psittaci*, *Chlamydia trichomatis*; *Escherichia coli*, *Haemophilus* species such as *Haemophilus influenza*; *Yersinia enterocolitica*; *Salmonella* species such as *S.typhimurium*; *Shigella* species such as *Shigella*

flexneri; *Streptococcus* species such as *S.agalactiae* and *S. pneumoniae*; *Bacilllus* species such as *Bacillus subtilis*; *Branhamella catarrhalis*; *Borrelia burgdorfer*; *Pseudomonas aeruginosa*; *Coxiella burnetti*; *Campylobacter* species such as *C.hyoilei*; *Helicobacter pylori*; and, *Klebsiella* species such as *Klebsiella pneumoniae*.

An inhibitor may also be used in the treatment of inflammatory diseases such as rheumatoid arthritis, asthma, inflammatory bowel disease, and atherosclerosis.

An inhibitor may also be used to augment the anti-cancer effects of agents such as interleukin-2 and poly-IC, to augment natural killer and macrophage tumoricidal activity, induce cytokine synthesis and secretion, enhance expression of LAK and HLA class I specific antigens; activate protein kinase C, stimulate bone marrow cell proliferation including hematopoietic progenitor cell proliferation, and increase engraftment efficiency and colony-forming unit activity, to confer protection against chemotherapy and radiation therapy (e.g. chemoprotective and radioprotective agents), and to accelerate recovery of bone marrow cellularity particularly when used in combination with chemical agents commonly used in the treatment of human diseases including cancer and acquired immune deficiency syndrome (AIDS). For example, an inhibitor can be used as a chemoprotectant in combination with anti-cancer agents including doxorubicin, 5-fluorouracil, cyclophosphamide, and methotrexate, and in combination with isoniazid or NSAID.

The present invention thus provides a method for treating the above-mentioned conditions in a subject comprising administering to a subject an effective amount of a modulator of the invention. The invention also contemplates a method for stimulating or inhibiting tumor growth or metastasis in a subject comprising administering to a subject an effective amount of a modulator of the invention.

The invention still further relates to a pharmaceutical composition which comprises a glycosyltransferase structure of the invention or a part thereof (e.g. an active site, a phosphate-binding loop lid, an SGC domain, DxD motif,), or a modulator of the invention in an amount effective to regulate one or more of the above-mentioned conditions (e.g. tumor growth or metastasis) and a pharmaceutically acceptable carrier, diluent or excipient.

The compositions of the invention are administered to subjects in a biologically compatible form suitable for pharmaceutical administration *in vivo*. By "biologically compatible form suitable for administration *in vivo*" is meant a form of the active ingredient to be administered in which any toxic effects are outweighed by the therapeutic effects of the active ingredient. The term "subject" is intended to include mammals and includes humans, dogs, cats, mice, rats, and transgenic species thereof. Administration of a therapeutically active amount of the pharmaceutical compositions of the present invention is defined as an amount effective, at dosages and for periods of time necessary to achieve the desired result. For example, a therapeutically active amount of a modulator of the invention may vary according to factors such as the condition, age, sex, and weight of the individual. Dosage regimes may be adjusted to provide the optimum therapeutic response. For example, several divided doses may be administered daily or the dose may be proportionally reduced as indicated by the exigencies of the therapeutic situation.

The active compound may be administered in a convenient manner such as by injection (subcutaneous, intravenous, etc.), oral administration, inhalation, transdermal application, or intracerebral administration.

A pharmaceutical composition of the invention can be administered to a subject in an appropriate carrier or diluent, co-administered with enzyme inhibitors or in an appropriate carrier such as microporous or solid beads or liposomes. The term "pharmaceutically acceptable carrier" as used herein is intended to include diluents such as saline and aqueous buffer solutions. Liposomes include water-in-oil-in-water emulsions as well as conventional liposomes (Strejan et al., (1984) J. Neuroimmunol 7:27). The active compound may also be administered parenterally or intraperitoneally. Dispersions can also be prepared in glycerol, liquid polyethylene glycols, and mixtures thereof and in oils. Under ordinary conditions of storage and use, these preparations may contain a preservative to prevent the growth of microorganisms. Depending on the route of administration, the active compound may be coated to protect the compound from the action of enzymes, acids, and other natural conditions which may inactivate the compound.

Therapeutic administration of polypeptide modulators may also be accomplished using gene therapy. A nucleic acid including a promoter operatively linked to a heterologous polypeptide may be used to produce high-level expression of the polypeptide in cells transfected with the nucleic acid. DNA or isolated nucleic acids may be introduced into cells of a subject by conventional nucleic acid delivery systems. Suitable delivery systems include liposomes, naked DNA, and receptor-mediated delivery systems, and viral vectors such as retroviruses, herpes viruses, and adenoviruses.

The following non-limiting examples are illustrative of the present invention:

EXAMPLE 1

Crystals of alpha-1,3-mannosyl-glycoprotein beta-1,2-N-acetylglucosaminyltransferase (GnT-1) were grown by the vapour-diffusion method from protein drops containing 10 mg/ml GnT-1, 10 mM MES buffer, pH 5.5, 270 mM KCL, 2-5 mM $MnCl_2$, and 10 mM UDP-GlcNAc, mixed with, and equilibrated against, 15-25% polyethylene glycol 8000, 100 mM Tris buffer, pH 7.9, 0 to 5% glycerol, and 0 to 10% isopropanol. Plate-like crystals grew within a few days, in space group $P2_12_12_1$ (a= 40.4 Å, b= 82.4Å, c= 102.5Å, $\alpha=\beta=\gamma=90°$), with one molecule in the asymmetric unit, and 40% solvent content.Data was collected from the crystals flash-frozen in a 100K N_2 stream, after a ten-minute wash with 21% polyethylene glycol 8000, 15% glycerol, and 100 mM Tris buffer, pH 7.9.

Atomic structural coordinates of an N-acetylglucosaminyltransferase I are set out in Table 1. Atomic coordinates of an N-acetylglucosaminyltransferase I with bound MeHg are set out in Table 2. The atomic structural coordinates of a rabbit N-acetylglucosaminyltransferase I bound to UDP-GlcNAc and a manganese 2+ ion are shown in Table 3. Atomic structural coordinates of an N-acetylglucosaminyltransferase I with acceptor are shown in Table 4. Figures 1 to 26, 28 to 30, and 32 to 40B illustrate glycosyltransferase structures, or binding sites or domains thereof.

EXAMPLE 2

The x-ray crystal structure of a soluble fragment containing the catalytic domain of a rabbit (Oryctolagus cuniculus) GnT I was determined at 1.4 Å resolution. The 342 residue catalytic domain of GnT I was expressed as an N-terminal histidine-tagged fusion protein (Sarker et al, Glycoconjugate J. 15:193-197, 1998), using the baculovirus/Sf9 system in a 3.5 litre bioreactor. The protein was purified using a CM HyperD F column, followed by a Ni-affinity column. The histidine tag was removed by enterokinase cleavage. Crystals were grown using the hanging-drop vapor diffusion method, from drops containing 10 mg/ml protein, 10 mM MES pH 6.5, 250 mM KCL, 2 mM $MnCl_2$, and 10 mM UDP-GlcNAc, and wells containing 17.5%-19.5% PEG 8000, 5% glycerol, and 100 mM Tris-HCl pH 7.9 Native and two-wavelength mercury-derivative data were collected using frozen crystals on the F2 beam line at the Cornell High Energy Synchrotron Source. The crystals grow in space group $P2_12_12_1$, with cell parameters a = 40.4 Å, b=82.4 Å, c = 102.5 Å. The structure was solved using the multiwavelength anomalous dispersion technique. GnTI contains both an eight-stranded mixed beta-sheet, flanked by six alpha helices, and a four-stranded mixed beta sheet, backed by three alpha helices. The structure reveals that the catalytic domain has dimensions 54 Å x 52 Å x 37 Å, with a large pocket on one face capable of holding both the UDP-GlcNAc donor and the Man_5Gn_2 acceptor. Sequence comparison shows that residues found in the pocket are very well conserved among GnT I sequences from different species. The pocket is flanked by a loop, not seen in the electron density map, which plays a role in either catalysis or substrate binding.

EXAMPLE 3

X-ray Crystal Structure of N-Acetylglucosaminyltransferase I: Structure, Mechanism, and the SGC Superfamily

Overall Structure

The catalytic fragment of rabbit GnT I (residues 106-447; Sarkar et al, 1998) was crystallized in the presence of UDP-GlcNAc and Mn^{2+}, and solved by the multi-wavelength anomalous diffraction (MAD) phasing method using a methylmercury chloride derivative (Table 6). In particular, crystals were grown using the hanging drop vapor diffusion method, by mixing equal 1.5 µl volumes of protein solution (10 mg/ml GnT I catalytic fragment, 10 mM MES buffer, pH 5.5, 270 mM KCl, 2 mM $MnCl_2$ and 10 mM UDP-GlcNAc) with well solution (15-25% polyethylene glycol 8000, 100 mM Tris buffer, pH 7.9, and 5% glycerol), and equilibrating against 1 ml of the well solution. A mercury derivative was obtained by soaking a crystal in well solution containing 20 mM MeHgCl. All data was collected using Quantum 4 charge-coupled device detectors on the F2 beamline of the Cornell High Energy Synchrotron Source, using crystals flash-frozen in the 100 K N_2 stream. Data were integrated, scaled, and reduced with DENZO and SCALEPACK (Otwinowski and Minor, 1997). The mercury position was identified with SOLVE (Terwilliger and Berendzen, 1999), and refined using SHARP (La Fortelle and Bricogne, 1997). Solvent flattening and histogram matching were

performed using DM (Cowtan, 1994). The resultant experimental map was traced using the program O (Jones et al, 1991), and the model refined with multiple rounds of manual rebuilding using O and OOPS2 (Kleywegt and Jones, 1996), alternated with simulated annealing and positional and B-factor refinement using CNS (Brunger et ak, 1998). The initial model was also refined against the "native" and "complex" data in a similar fashion.

In total, the structure was refined against data sets from 3 different crystals. Of these, no bound nucleotide sugar or Mn^{2+} ion was observed in the mercury "derivative" (refined at 1.4 Å resolution) nor in the structure refined against the data set that was termed "native" (1.5 Å resolution). Unlike that found in these *apo* structures, both components were seen in the "complex" (1.8 Å resolution). Since the native and derivative data sets were collected on samples that had aged before the x-ray data were collected, it was assumed that in these cases the UDP-GlcNAc had been hydrolysed.

GnT I is a two-domain protein, with overall dimensions of approximately 65 Å × 40 Å × 50 Å (Figure 25). The N-terminal domain (domain 1: residues 106-317) is an eight-stranded mixed β-sheet (β1-β8), flanked by six α-helices (α1-α6) and a small two-stranded antiparallel β-sheet (β4' and β8'). The smaller C-terminal domain (domain 2: residues 354-447) is a four-stranded mixed β-sheet (β9, β10, β13 and β14), flanked by three α-helices (α7-α9) and a short β-finger (β11 and β12). The two domains are connected by a linker region (residues 331 to 353) which wraps halfway around domain 1 before starting the first helix of domain 2. The ~1050 $Å^2$ interface between domain 1 and domain 2 is quite hydrophilic, and contains 20 bridging water molecules. The residues buried in the interface on domain 1 are 53% polar, while those in domain 2 are 36% polar.

The α-helices α3, α5 and α6 sit on "top" of the central β-sheet and create a pocket for the nucleotide-sugar and oligosaccharide acceptor. Electrostatic potential analysis shows that this pocket is largely acidic, in contrast to the rest of the protein surface, which is primarily positively charged. The nucleotide sugar itself sits between helicies α3 and α6 and β-strands β1, β2 and β4. The topology and structure of β-strands β1 to β4, and helices α1 to α3, are similar to those of the corresponding elements in domains possessing the Rossman fold, however, the orientation of the nucleotide sugar with respect to these elements is not.

In the native and derivative structures, in which UDP-GlcNAc and the Mn^{2+} ion were not observed, there is also no electron density for the 13-residue loop (residues 318-330) adjacent to the nucleotide-sugar binding site. The "missing loop" is presumed to be disordered in these crystals, as SDS-PAGE analysis of washed crystals showed the protein to be intact. These residues are structured in the complex, and are found to form a flap that partially covers the UDP-GlcNAc moiety. Although structured by UDP-GlcNAc binding only the tip of the loop makes direct interactions with it. Approximately 50 $Å^2$ is buried between the tip of the loop and the UDP-GlcNAc phosphates. Structuring the loop also buries ~600 $Å^2$ of protein surface adjacent to the nucleotide-sugar binding site. In these crystals the active site and the loop itself are exposed to a large solvent channel, and are not involved in crystal contacts. Aside from structuring the loop, there is no major conformational change associated with UDP-GlcNAc binding. The native and complex structures show a root-mean-squared-deviation (rmsd) of 0.28 Å, based on the α-carbon atoms of residues 106 to 317 and 331 to 447.

The Nucleotide Sugar and Metal Binding Sites

As shown by the structure of the complex, the UDP-GlcNAc is bound in the *anti* conformation. The uracil ring is sandwiched between I187 and the C115-C145 cysteine bridge, and its N3 and O2 make key hydrogen bond interactions with D144 and H190, respectively (Table 7 and Figure 33A). Moreover, its C5 is in van der Waals contact with V321, part of the loop structured by UDP-GlcNAc binding. The ribose O2' and O3' atoms make a water-mediated and a direct hydrogen bond, respectively, with the carboxyl side chain of D212. This Asp is the middle residue in the DXD motif common to a number of glycosyltransferases, as will be discussed in detail below.

The Mn^{2+} ion shows an octahedral geometry coordinated by six "inner-sphere" oxygen atoms (Table 7 and Figure 33B). The α- and β-phosphate of UDP-GlcNAc each contribute a coordinating oxygen atom, as do three water molecules. These water molecules are, in turn, hydrogen bonded to "outer sphere" protein residues E211, D213, T315 and G317. The remaining high-energy inner sphere metal ligand is provided by the carboxyl group of D213 -- the only direct interaction with the protein. As such, it seems that GnT I does not have an independent metal binding site capable of binding Mn^{2+} in the absence of UDP-GlcNAc. In addition to coordinating the Mn^{2+} ion, the phosphates make direct interactions with the protein. The α-phosphate makes a salt bridge with R117 and a hydrogen bond to the amide nitrogen of V321, and the β-phosphate hydrogen bonds to the hydroxyl group of S322. These interactions with V321 and S322 are an important component of the UDP-GlcNAc dependent structuring of the loop. Overall, the phosphates are in a conformation typical of divalent metal-bound nucleotides (Black et al, 1994).

Finally, the GlcNAc moiety itself makes several interactions with the protein (Table 7 and Figure 33C). The vicinal O3 and O4 hydroxyls are hydrogen bonded with the carboxyl group of E211 in a fashion seen in many lectin-carbohydrate complexes (Vyas, 1991). The O4 hydroxyl appears to play a central role, as it also makes a strong hydrogen bond with W290. The O6 hydroxyl is hydrogen bonded to a tightly bound water molecule seen in both the *apo* and complex structures. van der Waals interactions are also important, most notably between the *N*-acetyl methyl group and the side chains of L269 and L331.

The Glycosyltransferase DxD Motif

The DxD motif has been identified in many glycosyltransferase families and is thought to be involved in Mn^{2+} ion binding. The motif contains two Asp residues and is typically flanked by apolar residues (hhhhDxDxh) (Wiggins and Munro, 1998). (See Figures 27 and 31 for DxD motif alignments.) Site-directed mutagenesis has shown that both Asp's are required for yeast α-1,3-mannosyltransferase activity (Wiggins and Munro, 1998). In GnT I, the motif is present in a modified form (^{211}EDD^{213}), and with L214 forms the i to i+3 residues of a type 1 β-turn connecting β-strands β4 and β4' (Figure 39). As such, the highly conserved acidic residues are directed toward the same face of the turn. The fact that β4 runs through the core of the protein is consistent with the observed presence of several apolar residues on the N-terminal side of the motif.

The interactions with UDP-GlcNAc and the Mn^{2+} ion illustrate the importance of the motif. As discussed above, the second conserved Asp (D213) makes the only direct interaction with the bound Mn^{2+} ion. In addition, it makes a hydrogen bond with one of the metal coordinating water molecules, which itself is hydrogen bonded to the first conserved Asp (E211). Overall, these residues are conformationally constrained by the well-defined octahedral geometry characteristic of Mn^{2+} ion coordination. Since the phosphates of the

nucleotide sugar also coordinate the manganese ion, it serves to define the relative orientation of the nucleotide sugar and the conserved acid residues. In the case of GnT I this positions the GlcNAc moiety of the donor sugar for interaction with the first residue of the motif. In other sugar nucleoside diphosphate/Mn^{2+}-dependent glycosyltransferases, the first Asp of the DxD motif would be expected to play a carbohydrate-binding role, regardless of the nucleotide sugar type/linkage. It is well known that Asp is a key residue in carbohydrate binding proteins, and is thus well suited for such a role. Clearly, the well-conserved DxD motif does not simply serve to bind metal, but rather coordinates both the Mn^{2+} ion and the sugar moiety of the donor.

Reaction Mechanism

Catalysis by inverting glycosyltransferases is believed to involve a general base, such as Asp or Glu, which serves to assist in the deprotonation of the nucleophilic hydroxyl of the acceptor. In GnT I the only residue capable of playing this role is D291, 4.7 Å away from the GlcNAc C1 (Figure 33C). The structure shows that the acceptor will be able to approach the UDP-GlcNAc donor, so as to permit in-line nucleophilic attack and inversion of stereochemistry at the GlcNAc C1. Furthermore, the Mn^{2+} ion is disposed to pull developing negative charge away from the β-phosphate of the UDP leaving group (a role which may be aided by R117) (in which the hydration state of the ion is likely to play a crucial role (Cowan, 1998; Dudev et al, 1999).

Mechanistically, the reaction is thought to involve an oxocarbenium ion intermediate, similar to that proposed for glycosidases. Since glycosidases reduce the activation energy of the hydrolysis reaction by binding their substrates in a distorted conformation the GlcNAc ring conformation was examined for a similar effect. However, there was no evidence of significant distortion suggesting that the UDP-GlcNAc is bound in a low energy conformation: the sugar ring is a standard $^4C_1$ chair, and the glycosydic linkage is in an allowed conformation (Petrova et al 1999). As such, the UDP-GlcNAc is conceivably no more susceptible to nucleophilic attack by water than it would be in solution. Presumably, the activation energy for catalysis is derived from acceptor binding.

Loop Structuring and the Acceptor Binding Pocket

Comparison of the *apo* and complex structures shows that UDP-GlcNAc binding structures the 318-330 loop, forming a flap that partly covers the UDP-GlcNAc (Figure 40A). As discussed above V321 and S322, at the tip of the loop, make hydrogen bonds to the α- and β-phosphates of the UDP-GlcNAc. Residues 320-323 form a type IV turn, while the C-terminal residues 324-330 make one complete turn of an α-helix. The loop folds upon itself, burying residue F327 against R318 and the non-loop residues T315, L331 and K332. The only conformational changes other than structuring the loop itself are a peptide flip (F316-G317) and a reorientation of the T315 side chain. These changes are critical as the G317 carbonyl and the T315 hydroxyl are repositioned to make hydrogen bonds with two of the Mn^{2+} ion coordinating water molecules (see Figure 40A and Figure 33B).

As shown in Figure 40B, loop structuring creates a deep pocket, terminating over the proposed catalytic base (D291) and the GlcNAc moiety. The pocket itself can accommodate only a single monosaccharide residue of the $Man_5GlcNAc_2$ acceptor. One complete side of this pocket is formed by the loop structured upon UDP-GlcNAc binding. As a result two loop residues (S322 and F326), fully conserved among

active GnT I sequences, are presented to the acceptor binding pocket (Figure 40B). To explore the potential roles played by these and other residues in the binding pocket, a mannose residue was modeled into the site. With the attacking O2 hydroxyl positioned between the Asp 291 OE2 and the UDP-GlcNAc C1, only one general orientation leads to reasonable steric and chemical interactions with the protein. In this orientation, the exocyclic C6 hydroxymethyl group of the mannose interacts with S322 and F326, while the O3 and O4 point toward D291, R295 and R415.

The importance of the mannose O3, O4 and O6 predicted by this model is consistent with substrate studies using synthetic analogues of the trimannose core of the acceptor (Moller, 1992; Reck, 1995). In these studies it was further shown that even in the trimannose core, the known specificity of GnT I for the Manα1,3-arm over that of the Manα1,6-arm of the acceptor is preserved. This specificity is presumably dictated by interactions involving the β-mannose O4, the only other trisaccharide hydroxyl group found to be important. Extending the model to include all residues of the trimannose core (in its solution conformation) (Brisson and Cowen, 1983), the β-mannose O4 is positioned to interact with either D291 or D292. Similar interactions cannot be made when the 6-arm mannose is positioned in the binding pocket. Presumably the incoming nucleophile and associated binding energy serve to drive the reaction toward the transition state and ultimately product formation.

Enzyme Kinetics

Analysis has shown that GnT I proceeds through an ordered sequential Bi Bi kinetic mechanism (Nishikawa et al, 1988). The enzyme first binds Mn^{2+}/UDP-GlcNAc and then the $Man_5GlcNAc_2$ acceptor; the carbohydrate product is released first, followed by UDP. The GnT I structures provide an explanation for these observations. Since UDP-GlcNAc binding is required to structure the loop, and create the acceptor binding site, it is clear that the nucleotide sugar must bind first. Once catalysis has occurred, the UDP product cannot maintain the loop in its structured conformation, the acceptor binding pocket is destroyed, and the oligosaccharide product released. UDP, which is bound more weakly to GnT I than UDP-GlcNAc, is then free to diffuse out of the binding site, to be replaced by a fresh molecule of UDP-GlcNAc. By destroying the acceptor/product binding pocket, these kinetics also ensure that the enzyme is not strongly inhibited by the oligosaccharide product.

The structure also shows that GnT I does not itself have a Mn^{2+} ion binding site -- there is only a single direct protein-metal interaction. The Mn^{2+} ion is clearly more fully coordinated by UDP-GlcNAc, and positioned on the surface of the protein by virtue of its interactions with the nucleotide sugar. This mode of binding may also be an important determinant of how the enzyme releases its products. In the absence of an independent metal binding site, the UDP-Mn^{2+} complex would be free to dissociate from the enzyme surface, once catalysis has occurred.

The suggestion that bound UDP cannot support loop structuring stems from an analysis of the loop's interactions with UDP-GlcNAc in the complex. As discussed earlier, two residues (V321 and S322) at the tip of the loop form hydrogen bonds with oxygen atoms from the two phosphates. The loop's interactions are not otherwise very extensive, altogether burying only 50 $Å^2$ of the bound nucleotide sugar. Once the bond between the GlcNAc C1 and the β-phosphate oxygen is broken, the terminal phosphate acquires an additional

negative charge and presumably greater mobility (the latter enhanced by the lack of an independent Mn^{2+} ion binding site). Together, these effects would be expected to disrupt the ability of the phosphates to structure the loop. As such, it would seem that the structured loop can be thought of as a sensor for the integrity of the GlcNAc-phosphate linkage, thereby regulating formation and destruction of the acceptor/product binding site.

The SGC Domain

Analysis shows that the structure of domain 1 of GnT I is very similar to that of the *B. subtilis* glycosyltransferase spsA (residues 2-217) (Charnock and Davies, 1999). It possesses an identical topology, and all of the major secondary structural elements characterizing the domain are found in both structures (Figure 29). The domain is also found, with some modification in secondary structure (the topology remains the same), in β4Gal-T1 (residues 180-346) (Gastinel et al, 1999), and GlmU (residues 4-227, Figure 30) (Brown et al, 1999). Structural alignment using the program DALI, yields Z-scores of 15.7, 10.6 and 9.8, with spsA, β4Gal-T1 and GlmU, respectively. The very strong structural similarity between GnT I domain 1 and spsA suggests the existence of a canonical core domain, the SGC domain (spsA GnT I core domain), represented, in these four structures.

Despite the structural similarity shown by these enzymes, they do not show significant sequence similarity. Even with a knowledge of the structural alignment, GnT I shows only 10%, 12%, and 7% sequence identity with spsA, β4Gal-T1, and GlmU, respectively. These levels of identity make it difficult, if not impossible, to establish whether or not these enzymes stem from a common ancestor. Analysis of residues critical for function may, however, shed light on this question. The position of the UDP moiety in the GnT I complex is virtually identical to that found in the spsA complex (Figure 29) and is also very similar to that seen in the β4Gal-T1 and GlmU complexes. Moreover, the DxD motif is present in all four of these proteins and forms a perfectly superimposable type 1 β-turn in each case. Finally, at position D291, the proposed catalytic base in GnT I, both glycosyltransferases, spsA (D191) and β4Gal-T1 (D318), also possess Asp residues. Not only are these key residues and functional features identical in these structures, they are found at the same position on the structural/topological framework. The low sequence identity, common fold, and related functional features define the SGC superfamily, whose members are therefore likely to share a common evolutionary origin (Murzin et al, 1995).

The SGC Superfamily

The lack of sequence identity between glycosyltransferases with different specificities has lead to a classification that now includes 44 glycosyltransferase families. GnT I, for example, is in a family of its own, and a Position-Specific Iterated BLAST (PSI-BLAST) search, using the GnT I sequence, identifies no other related glycosyltransferases. Based on the knowledge that the GnT I SGC domain is structurally similar to spsA, an attempt was made at finding sequence similarity between these and other glycosyltransferases, thereby extending the SGC superfamily. The spsA sequence, coming from a much larger glycosyltransferase family, containing many divergent sequences, provides a more robust profile, and it was used to seed a PSI-BLAST search (Altschul et al, 1997). The search was able to identify similarity between spsA (family 2) and rabbit GnT I (family 13). It also showed similarity between spsA and the β-1,4-GalNAc transferases (family 12), the ceramide glucosyltransferases (family 21) and the polypeptide GalNAc transferases (family 27);

neither β4Gal-T1 (family 7), nor GlmU appeared in the searches.

To further explore possible relationships among the glycosyltransferase families, protein threading was used to determine the compatibility of a number of glycosyltransferase sequences with the SGC domain. Using the program THREADER 2, a single arbitrarily-selected sequence from each of the 27 glycosyltransferase families described by Campbell *et al.* (Campbell et al, 1998; Campbell et al, 1997) were run against a database of 1900 structures, which included the SGC domain of GnT I, spsA, β4Gal-T1 and GlmU. In both the normal and randomized test scores, the selected sequence from family 2, family 7, and family 13 ranked first or second against the SGC domain of spsA, β4Gal-T1 and GnT I, respectively, as would be expected. The sequence from family 3, family 6, family 16 and family 26 also ranked first or second in the two tests; sequences from several other families also received high scores. These results, and those based on PSI-BLAST searching, suggest that the SGC domain is widely represented among different families and includes both inverting and retaining glycosyltransferases.

Table 8 shows protein threading results. Proteins from different families were threaded against a THREADER 2 database containing 1900 protein folds, including GnT I, spsA, GlmU, and β4Gal-TI. The folds were sorted on the basis of their filtered combined energy Z-scores. When a GTCD-1-containing fold was one of the top thirty hits, out of 1900, then the top thirty hits were rerun with a randomization test of fifty shuffled-sequence threadings for each fold, to give a combined energy shuffled Z-score. A correct prediction should score well in both tests. Note that not only are inverting families represented, but so are retaining glycosyltransferases.

Conclusion

The structure of the catalytic domain of GnT I has provided the basis for its Mn^{2+}/UDP-GlcNAc binding properties, as well as insight into both its catalytic and kinetic mechanisms. The structure of the DxD motif shows that the first conserved residue plays a role in binding the donor sugar, while the second coordinates the essential Mn^{2+} ion. These roles are likely to be conserved in other DxD-containing glycosyltransferases, regardless of donor specificity. In addition, structural analysis has defined the SGC domain, seen in GnT I, spsA, β4Gal-T1 and GlmU. Sequence analysis and protein threading show that the SGC domain is contained in enzymes from several of the existing inverting and retaining glycosyltransferase families. Among these are enzymes involved in mammalian *N*- and *O*-linked oligosaccharide biosynthesis, bacterial cell wall production, and the synthesis of glycogen, chitin and cellulose. Together, they constitute the SGC superfamily.

Having illustrated and described the principles of the invention in a preferred embodiment, it should be appreciated to those skilled in the art that the invention can be modified in arrangement and detail without departure from such principles. All modifications coming within the scope of the following claims are claimed.

All publications, patents and patent applications referred to herein are incorporated by reference in their entirety to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated by reference in its entirety. In particular, U.S. provisional patent

applications Serial Nos. 60/139,949, filed June 18, 1999, 60/161,809, filed October 27, 1999, 60/178,401, filed January 27, 2000, and 60/202,509 filed May 5, 2000 are incorporated herein by reference.

Citations for References in the Specification

Altschul, S. F., Madden, T. L., Schaffer, A. A., Zhang, J., Zhang, Z., Miller, W., and Lipman, D. J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res *25*, 3389-402.

Bacon, D. J., and Anderson, W. F. (1988). A Fast Algorithm for Rendering Space-Filling Molecule Pictures. Journal of Molecular Graphics *6*, 219-220.

Black, C. B., Huang, H.-W., and Cowan, J. A. (1994). Biological coordination chemistry of magnesium, sodium, and potassium ions. Protein and nucleotide binding sites. Coordination Chemistry Reviews *135/136*, 165-202.

Brisson, J. R., and Carver, J. P. (1983). Solution conformation of alpha D(1-3)- and alpha D(1-6)-linked oligomannosides using proton nuclear magnetic resonance. Biochemistry *22*, 1362-8.

Brown, K., Pompeo, F., Dixon, S., Mengin-Lecreulx, D., Cambillau, C., and Bourne, Y. (1999). Crystal structure of the bifunctional N-acetylglucosamine 1-phosphate uridyltransferase from Escherichia coli: a paradigm for the related pyrophosphorylase superfamily. Embo J *18*, 4096-107.

Brunger, A. T., Adams, P. D., Clore, G. M., DeLano, W. L., Gros, P., Grosse-Kunstleve, R. W., Jiang, J. S., Kuszewski, J., Nilges, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T., and Warren, G. L. (1998). Crystallography & NMR system: A new software suite for macromolecular structure determination. Acta Crystallographica *D54*, 905-21.

Campbell, J. A., Davies, G. J., Bulone, V., and Henrissat, B. (1998). A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities. Biochem J *329*, 719.

Campbell, J. A., Davies, G. J., Bulone, V., and Henrissat, B. (1997). A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities [letter] [published erratum appears in Biochem J 1998 Feb 1;329(Pt 3):719]. Biochem J *326*, 929-39.

Charnock, S. J., and Davies, G. J. (1999). Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms. Biochemistry *38*, 6380-5.

Charuk, J. H., Tan, J., Bernardini, M., Haddad, S., Reithmeier, R. A., Jaeken, J., and Schachter, H. (1995). Carbohydrate-deficient glycoprotein syndrome type II. An autosomal recessive N-acetylglucosaminyltransferase II deficiency different from typical hereditary erythroblastic multinuclearity, with a positive acidified-serum lysis test (HEMPAS). Eur J Biochem *230*, 797-805.

Christopher, J. A. (1998). SPOCK: The Structural Properties Observation and Calculation Kit Program Manual. In SPOCK: The Structural Properties Observation and Calculation Kit Program Manual: The Center for Macromolecular Design, Texas A&M University, College Station, TX).

Coutinho, P. M., and Henrissat, B. (1999). Carbohydrate-Active Enzymes Server at URL: http://afmb.cnrs.mrs.fr/~pedro/CAZY/db.html. In Carbohydrate-Active Enzymes Server at URL: http://afmb.cnrs.mrs.fr/~pedro/CAZY/db.html.

Cowan, J. A. (1998). Magnesium activation of nuclease enzymes -- the importance of water. Inorganica Chimica Acta *275-276*, 24-7.

Cowtan, K. (1994). Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography *31*, 34-38.

Drickamer, K., and Taylor, M. E. (1998). Evolving views of protein glycosylation. Trends Biochem Sci *23*, 321-4.

Dudev, T., Cowan, J. A., and Lim, C. (1999). Competitive Binding in Magnesium Coordination Chemistry: Water versus Ligands of Biological Interest. J Am Chem Soc *121*, 7665-73.

Gastinel, L. N., Cambillau, C., and Bourne, Y. (1999). Crystal structures of the bovine beta4galactosyltransferase catalytic domain and its complex with uridine diphosphogalactose. Embo J *18*, 3546-57.

Granovsky, M., Fata, J., Pawling, J., Muller, W. J., Khokha, R., and Dennis, J. W. (2000). Suppression of tumor growth and metastasis in Mgat5-deficient mice. Nat Med *6*, 306-12.

Harpaz, N., and Schachter, H. (1980). Control of glycoprotein synthesis. Bovine colostrum UDP-N-acetylglucosamine:alpha-D-mannoside beta 2-N- acetylglucosaminyltransferase I. Separation from UDP-N-acetylglucosamine:alpha-D-mannoside beta 2-N- acetylglucosaminyltransferase II, partial purification, and substrate specificity. J Biol Chem *255*, 4885-93.

Ioffe, E., and Stanley, P. (1994). Mice lacking N-acetylglucosaminyltransferase I activity die at mid- gestation, revealing an essential role for complex or hybrid N-linked carbohydrates. Proc Natl Acad Sci U S A *91*, 728-32.

Jaeken, J., Carchon, H., and Stibler, H. (1993). The carbohydrate-deficient glycoprotein syndromes: pre-Golgi and Golgi disorders? Glycobiology *3*, 423-8.

Jaeken, J., Schachter, H., Carchon, H., De Cock, P., Coddeville, B., and Spik, G. (1994). Carbohydrate deficient glycoprotein syndrome type II: a deficiency in Golgi localised N-acetyl-glucosaminyltransferase II. Arch Dis Child *71*, 123-7.

Jones, T. A., Zou, J. Y., Cowan, S. W., and Kjeldgaard (1991). Improved methods for building protein models in electron density maps and the location of errors in these models. Acta Crystallographica *A47*, 110-119.

Kleywegt, G. J., and Jones, T. A. (1996). Efficient rebuilding of protein structures. Acta Crystallographica *D52*, 829-832.

Kornfeld, R., and Kornfeld, S. (1980). . In The Biochemistry of Glycoproteins and Proteoglycans, W. J. Lennarz, ed.: Plenum Press), pp. 24-25.

La Fortelle, E., and Bricogne, G. (1997). Maximum-Likelihood Heavy-Atom Parameter Refinement in the MIR and MAD Methods. Methods in Enzymology *276*, 472-494.

McCarter, J. D., and Withers, S. G. (1994). Mechanisms of enzymatic glycoside hydrolysis. Curr Opin Struct Biol *4*, 885-92.

Merritt, E. A., and Murphy, M. E. P. (1994). Raster3D Version 2.0, a Program for Photorealistic Molecular Graphics. Acta Crystallographica *D50*, 869-873.

Metzler, M., Gertz, A., Sarkar, M., Schachter, H., Schrader, J. W., and Marth, J. D. (1994). Complex asparagine-linked oligosaccharides are required for morphogenic events during post-implantation development. Embo J *13*, 2056-65.

Moller, G., Reck, F., Paulsen, H., Kaur, K. J., Sarkar, M., Schachter, H., and Brockhausen, I. (1992). Control of glycoprotein synthesis: substrate specificity of rat liver UDP-GlcNAc:Man alpha 3R beta 2-N-acetylglucosaminyltransferase I using synthetic substrate analogues. Glycoconj J *9*, 180-90.

Morera, S., Imberty, A., Aschke-Sonnenborn, U., Ruger, W., and Freemont, P. S. (1999). T4 phage beta-glucosyltransferase: substrate binding and proposed catalytic mechanism. J Mol Biol *292*, 717-30.

Murzin, A. G., Brenner, S. E., Hubbard, T., and Chothia, C. (1995). SCOP: a structural classification of proteins database for the investigation of sequences and structures. J Mol Biol *247*, 536-40.

Narasimhan, S., Stanley, P., and Schachter, H. (1977). Control of glycoprotein synthesis. Lectin-resistant

mutant containing only one of two distinct N-acetylglucosaminyltransferase activities present in wild type Chinese hamster ovary cells. J Biol Chem *252*, 3926-33.

Nishikawa, Y., Pegg, W., Paulsen, H., and Schachter, H. (1988). Control of glycoprotein synthesis. Purification and characterization of rabbit liver UDP-N-acetylglucosamine:alpha-3-D-mannoside beta-1,2-N-acetylglucosaminyltransferase I. J Biol Chem *263*, 8270-81.

Otwinowski, Z., and Minor, W. (1997). Processing of X-ray Diffraction Data Collected in Oscillation Mode. Methods in Enzymology *276*, 307-326.

Petrova, P., Koca, J., and Imberty, A. (1999). Potential Energy Hypersurfaces of Nucleotide Sugars: Ab Initio Calculations, Force-Field Parameterization, and Exploration of the Flexibility. J Am Chem Soc *121*, 5535-47.

Reck, F., Springer, M., Meinjohanns, E., Paulsen, H., Brockhausen, I., and Schachter, H. (1995). Synthetic substrate analogues for UDP-GlcNAc: Man alpha 1-3R beta 1-2-N- acetylglucosaminyltransferase I. Substrate specificity and inhibitors for the enzyme. Glycoconj J *12*, 747-54.

Reck, F., Springer, M., Paulsen, H., Brockhausen, I., Sarkar, M., and Schachter, H. (1994). Synthesis of tetrasaccharide analogues of the N-glycan substrate of beta-(1-->2)-N-acetylglucosaminyltransferase II using trisaccharide precursors and recombinant beta-(1-->2)-N-acetylglucosaminyltransferase I. Carbohydr Res *259*, 93-101.

Sarkar, M., Pagny, S., Unligil, U., Joziasse, D., Mucha, J., Glossl, J., and Schachter, H. (1998). Removal of 106 amino acids from the N-terminus of UDP-GlcNAc: alpha-3-D- mannoside beta-1,2-N-acetylglucosaminyltransferase I does not inactivate the enzyme. Glycoconj J *15*, 193-7.

Schachter, H. (1986). Biosynthetic controls that determine the branching and microheterogeneity of protein-bound oligosaccharides. Biochem Cell Biol *64*, 163-81.

Schachter, H. (1991). The 'yellow brick road' to branched complex N-glycans. Glycobiology *1*, 453-61.

Sinnott, M. L. (1991). Catalytic mechanisms of enzymic glycosyl transfer. Chem Rev *90*, 1170-1202.

Stanley, P., Narasimhan, S., Siminovitch, L., and Schachter, H. (1975). Chinese hamster ovary cells selected for resistance to the cytotoxicity of phytohemagglutinin are deficient in a UDP-N-acetylglucosamine--glycoprotein N-acetylglucosaminyltransferase activity. Proc Natl Acad Sci U S A *72*, 3323-7.

Tan, J., Dunn, J., Jaeken, J., and Schachter, H. (1996). Mutations in the MGAT2 gene controlling complex N-glycan synthesis cause carbohydrate-deficient glycoprotein syndrome type II, an autosomal recessive disease with defective brain development. Am J Hum Genet *59*, 810-7.

Terwilliger, T. C., and Berendzen, J. (1999). Automated MAD and MIR structure solution. Acta Crystallographica *D55*, 849-61.

Vrielink, A., Ruger, W., Driessen, H. P., and Freemont, P. S. (1994). Crystal structure of the DNA modifying enzyme beta-glucosyltransferase in the presence and absence of the substrate uridine diphosphoglucose. Embo J *13*, 3413-22.

Vyas, N. K. (1991). Atomic features of protein-carbohydrate interactions. Curr Opin Struct Biol *1*, 732-40.

Wiggins, C. A., and Munro, S. (1998). Activity of the yeast MNN1 alpha-1,3-mannosyltransferase requires a motif conserved in many other families of glycosyltransferases. Proc Natl Acad Sci U S A *95*, 7945-50.

Table 1

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REMARK GnT-1 native structure, "gntlg"
REMARK Ulug Unligil, 1999 06 14
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.5 A
REMARK starting r= .2186 free_r= .2322
REMARK final    r= .1991 free_r= .2154
REMARK B rmsd for bonded mainchain atoms=   .796  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  1.517  target= 2.0
REMARK B rmsd for angle mainchain atoms=  1.237  target= 2.0
REMARK B rmsd for angle sidechain atoms=  2.317  target= 2.5
REMARK wa= .685709
REMARK rweight=.167519
REMARK target= mlf  steps= 60
REMARK sg= P2(1)2(1)2(1) a= 40.478 b= 82.423 c= 102.480 alpha= 90 beta=
90 gamma= 90
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:water_rep.param
REMARK molecular structure file: generate_easy.mtf
REMARK input coordinates: bgroup.ann.pdb
REMARK reflection file= ../data/gntlg_start.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.5
REMARK initial B-factor correction applied to f_w3 :
REMARK   B11=   -.092 B22=   1.661 B33=  -1.569
REMARK   B12=    .000 B13=    .000 B23=    .000
REMARK B-factor correction applied to coordinate array B:    -.314
REMARK bulk solvent: density level= .380844 e/A^3, B-factor= 35.5223 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range:    106027 (
100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):   6093 (
5.7 % )
REMARK number of reflections rejected:                            0 (
.0 % )
REMARK total number of reflections used:                      99934 (
94.3 % )
REMARK number of reflections in working set:                  95035 (
89.6 % )
REMARK number of reflections in test set:                      4899 (
4.6 % )
REMARK FILENAME="bindividual.ann.pdb"
REMARK DATE:14-Jun-99  15:30:36       created by user: ulu
REMARK VERSION:0.5
ATOM      1  CB  LEU     0     -13.631  -6.605  17.468  1.00 25.79
ATOM      2  CG  LEU     0     -12.471  -7.459  18.001  1.00 26.76
ATOM      3  CD1 LEU     0     -13.039  -8.753  18.459  1.00 27.54
ATOM      4  CD2 LEU     0     -11.416  -7.693  16.934  1.00 27.20
ATOM      5  C   LEU     0     -15.350  -4.867  17.990  1.00 23.53
ATOM      6  O   LEU     0     -16.565  -5.005  17.847  1.00 24.56
ATOM      7  N   LEU     0     -15.395  -7.022  19.161  1.00 24.50
ATOM      8  CA  LEU     0     -14.509  -5.987  18.561  1.00 24.34
ATOM      9  N   ALA     1     -14.707  -3.754  17.665  1.00 21.34
ATOM     10  CA  ALA     1     -15.411  -2.598  17.140  1.00 20.20
ATOM     11  CB  ALA     1     -15.510  -1.546  18.223  1.00 19.83
ATOM     12  C   ALA     1     -14.714  -2.009  15.931  1.00 19.27
ATOM     13  O   ALA     1     -13.484  -2.106  15.804  1.00 19.08
```

ATOM	14	N	VAL	2	-15.494	-1.399	15.033	1.00	17.98
ATOM	15	CA	VAL	2	-14.897	-.758	13.857	1.00	17.00
ATOM	16	CB	VAL	2	-15.938	-.498	12.738	1.00	17.54
ATOM	17	CG1	VAL	2	-15.332	.431	11.673	1.00	17.84
ATOM	18	CG2	VAL	2	-16.344	-1.803	12.089	1.00	18.02
ATOM	19	C	VAL	2	-14.303	.587	14.298	1.00	15.19
ATOM	20	O	VAL	2	-14.982	1.395	14.939	1.00	15.36
ATOM	21	N	ILE	3	-13.025	.811	13.988	1.00	13.28
ATOM	22	CA	ILE	3	-12.339	2.053	14.344	1.00	12.37
ATOM	23	CB	ILE	3	-11.371	1.848	15.528	1.00	12.07
ATOM	24	CG2	ILE	3	-10.760	3.198	15.916	1.00	13.28
ATOM	25	CG1	ILE	3	-12.112	1.248	16.738	1.00	12.92
ATOM	26	CD1	ILE	3	-11.194	.870	17.910	1.00	13.59
ATOM	27	C	ILE	3	-11.528	2.530	13.135	1.00	11.57
ATOM	28	O	ILE	3	-10.518	1.924	12.768	1.00	11.18
ATOM	29	N	PRO	4	-11.957	3.627	12.501	1.00	9.75
ATOM	30	CD	PRO	4	-13.179	4.425	12.701	1.00	11.28
ATOM	31	CA	PRO	4	-11.208	4.107	11.341	1.00	9.18
ATOM	32	CB	PRO	4	-12.188	5.081	10.678	1.00	10.72
ATOM	33	CG	PRO	4	-12.913	5.649	11.859	1.00	10.86
ATOM	34	C	PRO	4	-9.891	4.781	11.702	1.00	9.00
ATOM	35	O	PRO	4	-9.721	5.340	12.799	1.00	8.03
ATOM	36	N	ILE	5	-8.948	4.692	10.774	1.00	7.89
ATOM	37	CA	ILE	5	-7.662	5.345	10.933	1.00	6.65
ATOM	38	CB	ILE	5	-6.493	4.427	10.543	1.00	7.18
ATOM	39	CG2	ILE	5	-5.181	5.166	10.756	1.00	7.45
ATOM	40	CG1	ILE	5	-6.537	3.117	11.346	1.00	6.82
ATOM	41	CD1	ILE	5	-6.516	3.288	12.831	1.00	6.56
ATOM	42	C	ILE	5	-7.736	6.513	9.936	1.00	8.13
ATOM	43	O	ILE	5	-7.964	6.313	8.737	1.00	8.40
ATOM	44	N	LEU	6	-7.573	7.731	10.433	1.00	6.77
ATOM	45	CA	LEU	6	-7.634	8.911	9.587	1.00	7.04
ATOM	46	CB	LEU	6	-8.487	9.994	10.245	1.00	7.61
ATOM	47	CG	LEU	6	-8.435	11.365	9.570	1.00	7.30
ATOM	48	CD1	LEU	6	-9.006	11.298	8.121	1.00	9.38
ATOM	49	CD2	LEU	6	-9.213	12.344	10.435	1.00	9.39
ATOM	50	C	LEU	6	-6.211	9.402	9.453	1.00	6.65
ATOM	51	O	LEU	6	-5.638	9.869	10.416	1.00	6.58
ATOM	52	N	VAL	7	-5.650	9.277	8.259	1.00	7.02
ATOM	53	CA	VAL	7	-4.278	9.701	7.996	1.00	6.76
ATOM	54	CB	VAL	7	-3.601	8.724	6.987	1.00	6.41
ATOM	55	CG1	VAL	7	-2.222	9.199	6.617	1.00	6.69
ATOM	56	CG2	VAL	7	-3.544	7.324	7.578	1.00	7.07
ATOM	57	C	VAL	7	-4.280	11.118	7.417	1.00	7.27
ATOM	58	O	VAL	7	-4.969	11.392	6.424	1.00	7.47
ATOM	59	N	ILE	8	-3.495	12.004	8.036	1.00	8.30
ATOM	60	CA	ILE	8	-3.382	13.399	7.622	1.00	8.20
ATOM	61	CB	ILE	8	-3.246	14.325	8.844	1.00	9.09
ATOM	62	CG2	ILE	8	-3.187	15.786	8.382	1.00	8.34
ATOM	63	CG1	ILE	8	-4.414	14.102	9.804	1.00	8.57
ATOM	64	CD1	ILE	8	-5.772	14.412	9.200	1.00	10.81
ATOM	65	C	ILE	8	-2.159	13.572	6.740	1.00	9.52
ATOM	66	O	ILE	8	-1.029	13.487	7.220	1.00	9.86
ATOM	67	N	ALA	9	-2.395	13.835	5.456	1.00	10.12
ATOM	68	CA	ALA	9	-1.316	13.988	4.481	1.00	11.14
ATOM	69	CB	ALA	9	-1.363	12.837	3.496	1.00	12.45
ATOM	70	C	ALA	9	-1.399	15.296	3.718	1.00	12.53
ATOM	71	O	ALA	9	-2.424	15.961	3.715	1.00	11.47
ATOM	72	N	CYS	10	-.303	15.641	3.055	1.00	14.91
ATOM	73	CA	CYS	10	-.259	16.863	2.266	1.00	17.11

ATOM	74	C	CYS	10	.732	16.804	1.100	1.00	17.11
ATOM	75	O	CYS	10	.344	16.448	-.030	1.00	17.71
ATOM	76	CB	CYS	10	.009	18.054	3.186	1.00	19.21
ATOM	77	SG	CYS	10	.633	19.609	2.456	1.00	22.63
ATOM	78	N	ASP	11	1.997	17.140	1.339	1.00	18.08
ATOM	79	CA	ASP	11	2.966	17.142	.244	1.00	18.18
ATOM	80	CB	ASP	11	3.301	18.590	-.138	1.00	19.24
ATOM	81	CG	ASP	11	3.700	19.437	1.061	1.00	19.48
ATOM	82	OD1	ASP	11	3.891	20.668	.892	1.00	20.34
ATOM	83	OD2	ASP	11	3.839	18.884	2.178	1.00	19.92
ATOM	84	C	ASP	11	4.258	16.365	.467	1.00	18.74
ATOM	85	O	ASP	11	5.323	16.777	.005	1.00	18.41
ATOM	86	N	ARG	12	4.170	15.251	1.186	1.00	18.46
ATOM	87	CA	ARG	12	5.330	14.411	1.427	1.00	18.31
ATOM	88	CB	ARG	12	5.634	14.366	2.925	1.00	20.13
ATOM	89	CG	ARG	12	6.000	15.736	3.491	1.00	22.63
ATOM	90	CD	ARG	12	6.129	15.715	5.025	1.00	25.97
ATOM	91	NE	ARG	12	7.178	14.808	5.490	1.00	29.63
ATOM	92	CZ	ARG	12	7.464	14.580	6.778	1.00	31.55
ATOM	93	NH1	ARG	12	6.777	15.198	7.741	1.00	32.76
ATOM	94	NH2	ARG	12	8.426	13.718	7.107	1.00	32.39
ATOM	95	C	ARG	12	5.026	13.026	.872	1.00	17.56
ATOM	96	O	ARG	12	4.117	12.334	1.349	1.00	17.66
ATOM	97	N	SER	13	5.784	12.634	-.148	1.00	16.84
ATOM	98	CA	SER	13	5.607	11.339	-.800	1.00	16.27
ATOM	99	CB	SER	13	6.530	11.225	-2.018	1.00	17.27
ATOM	100	OG	SER	13	7.886	11.190	-1.628	1.00	19.04
ATOM	101	C	SER	13	5.859	10.176	.152	1.00	15.57
ATOM	102	O	SER	13	5.413	9.039	-.110	1.00	13.53
ATOM	103	N	THR	14	6.550	10.465	1.259	1.00	14.21
ATOM	104	CA	THR	14	6.841	9.451	2.269	1.00	15.22
ATOM	105	CB	THR	14	8.002	9.903	3.218	1.00	15.24
ATOM	106	OG1	THR	14	7.753	11.227	3.698	1.00	17.08
ATOM	107	CG2	THR	14	9.356	9.886	2.474	1.00	15.93
ATOM	108	C	THR	14	5.595	9.026	3.084	1.00	14.60
ATOM	109	O	THR	14	5.685	8.263	4.058	1.00	14.63
ATOM	110	N	VAL	15	4.418	9.506	2.674	1.00	13.82
ATOM	111	CA	VAL	15	3.176	9.067	3.312	1.00	11.94
ATOM	112	CB	VAL	15	1.907	9.783	2.724	1.00	11.62
ATOM	113	CG1	VAL	15	1.802	9.577	1.213	1.00	11.91
ATOM	114	CG2	VAL	15	.654	9.237	3.404	1.00	12.94
ATOM	115	C	VAL	15	3.152	7.564	2.964	1.00	11.02
ATOM	116	O	VAL	15	2.453	6.770	3.580	1.00	10.98
ATOM	117	N	ARG	16	3.940	7.192	1.956	1.00	10.63
ATOM	118	CA	ARG	16	4.060	5.799	1.522	1.00	9.47
ATOM	119	CB	ARG	16	5.072	5.679	.363	1.00	10.28
ATOM	120	CG	ARG	16	5.356	4.221	-.077	1.00	10.39
ATOM	121	CD	ARG	16	6.429	4.127	-1.176	1.00	12.00
ATOM	122	NE	ARG	16	6.027	4.785	-2.422	1.00	12.95
ATOM	123	CZ	ARG	16	5.223	4.257	-3.346	1.00	13.63
ATOM	124	NH1	ARG	16	4.716	3.049	-3.174	1.00	13.73
ATOM	125	NH2	ARG	16	4.964	4.917	-4.474	1.00	13.90
ATOM	126	C	ARG	16	4.511	4.896	2.671	1.00	9.78
ATOM	127	O	ARG	16	3.973	3.808	2.857	1.00	10.24
ATOM	128	N	ARG	17	5.518	5.338	3.421	1.00	9.80
ATOM	129	CA	ARG	17	6.048	4.560	4.537	1.00	9.85
ATOM	130	CB	ARG	17	7.312	5.230	5.084	1.00	11.01
ATOM	131	CG	ARG	17	7.861	4.607	6.372	1.00	13.22
ATOM	132	CD	ARG	17	9.219	5.196	6.762	1.00	15.90
ATOM	133	NE	ARG	17	9.688	4.748	8.081	1.00	17.33

ATOM	134	CZ	ARG	17	10.812	5.184	8.654	1.00	17.86
ATOM	135	NH1	ARG	17	11.579	6.068	8.025	1.00	17.86
ATOM	136	NH2	ARG	17	11.164	4.754	9.862	1.00	18.56
ATOM	137	C	ARG	17	5.020	4.418	5.643	1.00	9.79
ATOM	138	O	ARG	17	4.911	3.359	6.284	1.00	9.50
ATOM	139	N	CYS	18	4.274	5.496	5.867	1.00	9.21
ATOM	140	CA	CYS	18	3.235	5.518	6.887	1.00	8.90
ATOM	141	CB	CYS	18	2.620	6.919	6.983	1.00	8.64
ATOM	142	SG	CYS	18	1.181	7.076	8.104	1.00	8.71
ATOM	143	C	CYS	18	2.160	4.503	6.512	1.00	8.53
ATOM	144	O	CYS	18	1.811	3.650	7.319	1.00	8.11
ATOM	145	N	LEU	19	1.655	4.585	5.284	1.00	7.80
ATOM	146	CA	LEU	19	.623	3.655	4.836	1.00	7.57
ATOM	147	CB	LEU	19	.054	4.084	3.479	1.00	7.84
ATOM	148	CG	LEU	19	-.761	5.385	3.471	1.00	9.37
ATOM	149	CD1	LEU	19	-1.151	5.768	2.029	1.00	10.39
ATOM	150	CD2	LEU	19	-2.016	5.213	4.322	1.00	9.86
ATOM	151	C	LEU	19	1.110	2.209	4.764	1.00	7.26
ATOM	152	O	LEU	19	.375	1.283	5.113	1.00	7.22
ATOM	153	N	ASP	20	2.341	1.993	4.320	1.00	8.26
ATOM	154	CA	ASP	20	2.830	.627	4.244	1.00	8.53
ATOM	155	CB	ASP	20	4.244	.570	3.661	1.00	9.68
ATOM	156	CG	ASP	20	4.293	.865	2.159	1.00	12.09
ATOM	157	OD1	ASP	20	3.253	.849	1.457	1.00	12.42
ATOM	158	OD2	ASP	20	5.418	1.097	1.673	1.00	13.96
ATOM	159	C	ASP	20	2.823	-.048	5.607	1.00	8.84
ATOM	160	O	ASP	20	2.454	-1.211	5.709	1.00	8.44
ATOM	161	N	LYS	21	3.240	.661	6.656	1.00	9.49
ATOM	162	CA	LYS	21	3.240	.043	7.978	1.00	9.86
ATOM	163	CB	LYS	21	4.041	.894	8.961	1.00	12.07
ATOM	164	CG	LYS	21	5.507	.985	8.617	1.00	14.76
ATOM	165	CD	LYS	21	6.197	-.327	8.886	1.00	16.57
ATOM	166	CE	LYS	21	7.673	-.284	8.452	1.00	18.48
ATOM	167	NZ	LYS	21	8.342	-1.565	8.833	1.00	22.07
ATOM	168	C	LYS	21	1.825	-.190	8.511	1.00	9.34
ATOM	169	O	LYS	21	1.537	-1.245	9.085	1.00	9.51
ATOM	170	N	LEU	22	.937	.788	8.329	1.00	8.52
ATOM	171	CA	LEU	22	-.444	.640	8.784	1.00	7.38
ATOM	172	CB	LEU	22	-1.260	1.868	8.414	1.00	7.50
ATOM	173	CG	LEU	22	-1.045	3.085	9.305	1.00	6.56
ATOM	174	CD1	LEU	22	-1.498	4.336	8.570	1.00	8.17
ATOM	175	CD2	LEU	22	-1.799	2.906	10.610	1.00	7.61
ATOM	176	C	LEU	22	-1.080	-.576	8.119	1.00	8.79
ATOM	177	O	LEU	22	-1.701	-1.411	8.789	1.00	8.82
ATOM	178	N	LEU	23	-.913	-.658	6.801	1.00	8.44
ATOM	179	CA	LEU	23	-1.474	-1.740	6.008	1.00	8.55
ATOM	180	CB	LEU	23	-1.312	-1.416	4.515	1.00	9.19
ATOM	181	CG	LEU	23	-2.307	-.333	4.082	1.00	9.05
ATOM	182	CD1	LEU	23	-1.955	.235	2.711	1.00	10.05
ATOM	183	CD2	LEU	23	-3.699	-.936	4.079	1.00	10.26
ATOM	184	C	LEU	23	-.864	-3.094	6.338	1.00	9.60
ATOM	185	O	LEU	23	-1.561	-4.107	6.315	1.00	10.66
ATOM	186	N	HIS	24	.430	-3.113	6.631	1.00	8.87
ATOM	187	CA	HIS	24	1.111	-4.352	6.977	1.00	9.68
ATOM	188	CB	HIS	24	2.612	-4.098	7.064	1.00	10.68
ATOM	189	CG	HIS	24	3.392	-5.292	7.508	1.00	12.77
ATOM	190	CD2	HIS	24	3.865	-5.640	8.727	1.00	14.51
ATOM	191	ND1	HIS	24	3.687	-6.341	6.665	1.00	16.15
ATOM	192	CE1	HIS	24	4.310	-7.286	7.348	1.00	15.95
ATOM	193	NE2	HIS	24	4.429	-6.886	8.602	1.00	16.73

ATOM	194	C	HIS	24	.614	-4.937	8.313	1.00	9.79
ATOM	195	O	HIS	24	.383	-6.147	8.443	1.00	11.44
ATOM	196	N	TYR	25	.440	-4.073	9.301	1.00	9.30
ATOM	197	CA	TYR	25	.008	-4.513	10.622	1.00	9.66
ATOM	198	CB	TYR	25	.694	-3.649	11.694	1.00	9.28
ATOM	199	CG	TYR	25	2.168	-3.973	11.839	1.00	11.37
ATOM	200	CD1	TYR	25	3.135	-2.981	11.771	1.00	12.61
ATOM	201	CE1	TYR	25	4.492	-3.295	11.912	1.00	14.29
ATOM	202	CD2	TYR	25	2.587	-5.287	12.050	1.00	11.88
ATOM	203	CE2	TYR	25	3.921	-5.607	12.192	1.00	14.23
ATOM	204	CZ	TYR	25	4.872	-4.616	12.126	1.00	14.70
ATOM	205	OH	TYR	25	6.205	-4.941	12.293	1.00	17.45
ATOM	206	C	TYR	25	-1.491	-4.564	10.862	1.00	10.09
ATOM	207	O	TYR	25	-1.943	-5.149	11.845	1.00	10.62
ATOM	208	N	ARG	26	-2.263	-3.967	9.968	1.00	9.63
ATOM	209	CA	ARG	26	-3.712	-3.958	10.121	1.00	10.57
ATOM	210	CB	ARG	26	-4.353	-3.199	8.958	1.00	11.25
ATOM	211	CG	ARG	26	-5.854	-3.247	8.966	1.00	10.62
ATOM	212	CD	ARG	26	-6.486	-2.186	8.068	1.00	10.74
ATOM	213	NE	ARG	26	-6.376	-2.475	6.637	1.00	10.97
ATOM	214	CZ	ARG	26	-7.069	-1.816	5.707	1.00	9.81
ATOM	215	NH1	ARG	26	-7.901	-.854	6.066	1.00	10.36
ATOM	216	NH2	ARG	26	-6.930	-2.119	4.425	1.00	11.47
ATOM	217	C	ARG	26	-4.247	-5.384	10.178	1.00	10.63
ATOM	218	O	ARG	26	-3.992	-6.178	9.288	1.00	10.67
ATOM	219	N	PRO	27	-5.015	-5.718	11.222	1.00	10.67
ATOM	220	CD	PRO	27	-5.268	-4.974	12.469	1.00	10.84
ATOM	221	CA	PRO	27	-5.534	-7.086	11.309	1.00	11.81
ATOM	222	CB	PRO	27	-5.850	-7.231	12.783	1.00	11.66
ATOM	223	CG	PRO	27	-6.271	-5.854	13.177	1.00	11.48
ATOM	224	C	PRO	27	-6.749	-7.354	10.447	1.00	13.14
ATOM	225	O	PRO	27	-6.969	-8.491	10.007	1.00	14.56
ATOM	226	N	SER	28	-7.517	-6.299	10.187	1.00	13.61
ATOM	227	CA	SER	28	-8.742	-6.394	9.420	1.00	14.74
ATOM	228	CB	SER	28	-9.868	-6.767	10.398	1.00	15.26
ATOM	229	OG	SER	28	-11.145	-6.614	9.836	1.00	16.22
ATOM	230	C	SER	28	-9.074	-5.084	8.698	1.00	14.30
ATOM	231	O	SER	28	-9.076	-4.013	9.324	1.00	14.12
ATOM	232	N	ALA	29	-9.356	-5.158	7.396	1.00	14.27
ATOM	233	CA	ALA	29	-9.724	-3.964	6.646	1.00	14.41
ATOM	234	CB	ALA	29	-9.739	-4.240	5.136	1.00	15.51
ATOM	235	C	ALA	29	-11.108	-3.528	7.100	1.00	14.87
ATOM	236	O	ALA	29	-11.443	-2.352	7.048	1.00	15.67
ATOM	237	N	GLU	30	-11.923	-4.478	7.543	1.00	15.14
ATOM	238	CA	GLU	30	-13.260	-4.139	7.991	1.00	16.02
ATOM	239	CB	GLU	30	-14.111	-5.397	8.104	1.00	19.20
ATOM	240	CG	GLU	30	-14.257	-6.208	6.836	1.00	23.18
ATOM	241	CD	GLU	30	-14.813	-7.586	7.158	1.00	25.96
ATOM	242	OE1	GLU	30	-14.021	-8.569	7.271	1.00	27.22
ATOM	243	OE2	GLU	30	-16.053	-7.684	7.331	1.00	27.72
ATOM	244	C	GLU	30	-13.249	-3.442	9.342	1.00	14.64
ATOM	245	O	GLU	30	-14.007	-2.510	9.565	1.00	14.99
ATOM	246	N	LEU	31	-12.393	-3.899	10.251	1.00	14.77
ATOM	247	CA	LEU	31	-12.331	-3.312	11.580	1.00	14.69
ATOM	248	CB	LEU	31	-11.670	-4.291	12.546	1.00	16.96
ATOM	249	CG	LEU	31	-12.547	-4.824	13.671	1.00	20.11
ATOM	250	CD1	LEU	31	-13.934	-5.124	13.147	1.00	21.16
ATOM	251	CD2	LEU	31	-11.908	-6.052	14.237	1.00	20.82
ATOM	252	C	LEU	31	-11.587	-1.988	11.623	1.00	13.40
ATOM	253	O	LEU	31	-11.889	-1.138	12.456	1.00	13.29

ATOM	254	N	PHE	32	-10.618	-1.822	10.725	1.00	11.41
ATOM	255	CA	PHE	32	-9.833	-.599	10.674	1.00	10.55
ATOM	256	CB	PHE	32	-8.421	-.856	11.189	1.00	9.91
ATOM	257	CG	PHE	32	-8.368	-1.196	12.650	1.00	10.80
ATOM	258	CD1	PHE	32	-8.321	-2.519	13.071	1.00	11.72
ATOM	259	CD2	PHE	32	-8.384	-.186	13.605	1.00	11.68
ATOM	260	CE1	PHE	32	-8.291	-2.832	14.433	1.00	13.77
ATOM	261	CE2	PHE	32	-8.350	-.504	14.960	1.00	13.74
ATOM	262	CZ	PHE	32	-8.305	-1.820	15.368	1.00	13.29
ATOM	263	C	PHE	32	-9.751	.027	9.289	1.00	10.03
ATOM	264	O	PHE	32	-8.702	-.020	8.638	1.00	10.49
ATOM	265	N	PRO	33	-10.856	.622	8.813	1.00	10.24
ATOM	266	CD	PRO	33	-12.154	.850	9.467	1.00	11.10
ATOM	267	CA	PRO	33	-10.815	1.248	7.482	1.00	10.53
ATOM	268	CB	PRO	33	-12.243	1.750	7.272	1.00	11.07
ATOM	269	CG	PRO	33	-13.052	1.023	8.304	1.00	13.72
ATOM	270	C	PRO	33	-9.836	2.407	7.555	1.00	10.35
ATOM	271	O	PRO	33	-9.776	3.103	8.570	1.00	10.33
ATOM	272	N	ILE	34	-9.068	2.607	6.492	1.00	9.09
ATOM	273	CA	ILE	34	-8.091	3.685	6.458	1.00	9.12
ATOM	274	CB	ILE	34	-6.715	3.152	6.022	1.00	8.63
ATOM	275	CG2	ILE	34	-5.733	4.310	5.791	1.00	10.16
ATOM	276	CG1	ILE	34	-6.199	2.169	7.082	1.00	9.56
ATOM	277	CD1	ILE	34	-5.022	1.382	6.635	1.00	10.25
ATOM	278	C	ILE	34	-8.562	4.756	5.489	1.00	8.52
ATOM	279	O	ILE	34	-8.839	4.468	4.335	1.00	10.14
ATOM	280	N	ILE	35	-8.699	5.978	5.989	1.00	8.70
ATOM	281	CA	ILE	35	-9.132	7.108	5.178	1.00	8.10
ATOM	282	CB	ILE	35	-10.347	7.828	5.817	1.00	8.86
ATOM	283	CG2	ILE	35	-10.624	9.165	5.115	1.00	9.16
ATOM	284	CG1	ILE	35	-11.568	6.894	5.783	1.00	10.58
ATOM	285	CD1	ILE	35	-11.497	5.786	6.803	1.00	12.13
ATOM	286	C	ILE	35	-7.964	8.065	5.164	1.00	8.31
ATOM	287	O	ILE	35	-7.512	8.472	6.219	1.00	8.37
ATOM	288	N	VAL	36	-7.465	8.392	3.976	1.00	7.05
ATOM	289	CA	VAL	36	-6.345	9.310	3.834	1.00	7.86
ATOM	290	CB	VAL	36	-5.295	8.803	2.827	1.00	7.81
ATOM	291	CG1	VAL	36	-4.056	9.694	2.894	1.00	9.16
ATOM	292	CG2	VAL	36	-4.923	7.356	3.133	1.00	8.97
ATOM	293	C	VAL	36	-6.878	10.635	3.333	1.00	7.94
ATOM	294	O	VAL	36	-7.406	10.718	2.219	1.00	8.57
ATOM	295	N	SER	37	-6.763	11.654	4.176	1.00	7.82
ATOM	296	CA	SER	37	-7.206	12.991	3.817	1.00	8.88
ATOM	297	CB	SER	37	-7.846	13.686	5.020	1.00	8.09
ATOM	298	OG	SER	37	-8.356	14.958	4.648	1.00	9.70
ATOM	299	C	SER	37	-5.961	13.734	3.380	1.00	9.22
ATOM	300	O	SER	37	-5.010	13.895	4.152	1.00	8.67
ATOM	301	N	GLN	38	-5.970	14.182	2.128	1.00	9.11
ATOM	302	CA	GLN	38	-4.835	14.887	1.571	1.00	9.92
ATOM	303	CB	GLN	38	-4.420	14.260	.242	1.00	11.23
ATOM	304	CG	GLN	38	-3.026	14.665	-.211	1.00	11.96
ATOM	305	CD	GLN	38	-2.805	14.523	-1.697	1.00	13.01
ATOM	306	OE1	GLN	38	-3.521	13.787	-2.389	1.00	14.20
ATOM	307	NE2	GLN	38	-1.793	15.224	-2.201	1.00	12.66
ATOM	308	C	GLN	38	-5.175	16.345	1.310	1.00	11.32
ATOM	309	O	GLN	38	-6.152	16.641	.623	1.00	11.97
ATOM	310	N	ASP	39	-4.350	17.237	1.843	1.00	11.62
ATOM	311	CA	ASP	39	-4.514	18.672	1.657	1.00	12.97
ATOM	312	CB	ASP	39	-4.312	19.363	3.010	1.00	12.01
ATOM	313	CG	ASP	39	-4.673	20.831	2.993	1.00	13.11

ATOM	314	OD1	ASP	39	-5.304	21.292	2.023	1.00	11.56
ATOM	315	OD2	ASP	39	-4.332	21.518	3.985	1.00	14.44
ATOM	316	C	ASP	39	-3.401	19.074	.685	1.00	15.29
ATOM	317	O	ASP	39	-2.597	18.219	.272	1.00	15.02
ATOM	318	N	CYS	40	-3.388	20.344	.267	1.00	16.62
ATOM	319	CA	CYS	40	-2.311	20.860	-.583	1.00	19.90
ATOM	320	C	CYS	40	-2.261	20.568	-2.080	1.00	19.96
ATOM	321	O	CYS	40	-1.562	21.275	-2.829	1.00	21.14
ATOM	322	CB	CYS	40	-.984	20.434	.027	1.00	20.94
ATOM	323	SG	CYS	40	-.946	20.704	1.816	1.00	24.90
ATOM	324	N	GLY	41	-2.958	19.536	-2.530	1.00	20.40
ATOM	325	CA	GLY	41	-2.932	19.218	-3.951	1.00	20.66
ATOM	326	C	GLY	41	-1.537	18.989	-4.506	1.00	20.80
ATOM	327	O	GLY	41	-1.169	19.526	-5.554	1.00	21.70
ATOM	328	N	HIS	42	-.730	18.218	-3.794	1.00	20.08
ATOM	329	CA	HIS	42	.615	17.897	-4.248	1.00	19.01
ATOM	330	CB	HIS	42	1.502	17.593	-3.035	1.00	18.75
ATOM	331	CG	HIS	42	2.935	17.338	-3.376	1.00	19.03
ATOM	332	CD2	HIS	42	3.986	18.181	-3.509	1.00	19.57
ATOM	333	ND1	HIS	42	3.426	16.074	-3.600	1.00	18.85
ATOM	334	CE1	HIS	42	4.721	16.144	-3.853	1.00	20.66
ATOM	335	NE2	HIS	42	5.087	17.413	-3.801	1.00	20.10
ATOM	336	C	HIS	42	.403	16.679	-5.148	1.00	19.31
ATOM	337	O	HIS	42	-.013	15.607	-4.692	1.00	17.46
ATOM	338	N	GLU	43	.631	16.862	-6.445	1.00	20.11
ATOM	339	CA	GLU	43	.412	15.815	-7.438	1.00	21.05
ATOM	340	CB	GLU	43	.845	16.319	-8.817	1.00	23.65
ATOM	341	CG	GLU	43	-.013	15.796	-9.944	1.00	27.05
ATOM	342	CD	GLU	43	-1.477	15.734	-9.552	1.00	29.62
ATOM	343	OE1	GLU	43	-2.054	16.794	-9.178	1.00	31.53
ATOM	344	OE2	GLU	43	-2.063	14.624	-9.602	1.00	31.40
ATOM	345	C	GLU	43	1.050	14.463	-7.181	1.00	20.19
ATOM	346	O	GLU	43	.363	13.438	-7.218	1.00	20.47
ATOM	347	N	GLU	44	2.357	14.457	-6.934	1.00	20.21
ATOM	348	CA	GLU	44	3.091	13.221	-6.704	1.00	20.34
ATOM	349	CB	GLU	44	4.573	13.527	-6.463	1.00	23.01
ATOM	350	CG	GLU	44	5.199	14.365	-7.589	1.00	26.78
ATOM	351	CD	GLU	44	4.606	15.775	-7.689	1.00	28.87
ATOM	352	OE1	GLU	44	4.898	16.599	-6.794	1.00	29.85
ATOM	353	OE2	GLU	44	3.831	16.071	-8.651	1.00	30.49
ATOM	354	C	GLU	44	2.494	12.470	-5.519	1.00	18.80
ATOM	355	O	GLU	44	2.336	11.253	-5.548	1.00	18.40
ATOM	356	N	THR	45	2.140	13.201	-4.472	1.00	17.18
ATOM	357	CA	THR	45	1.560	12.570	-3.299	1.00	15.14
ATOM	358	CB	THR	45	1.446	13.569	-2.149	1.00	14.39
ATOM	359	OG1	THR	45	2.751	14.027	-1.787	1.00	14.89
ATOM	360	CG2	THR	45	.799	12.916	-.938	1.00	14.92
ATOM	361	C	THR	45	.183	11.986	-3.627	1.00	14.94
ATOM	362	O	THR	45	-.169	10.913	-3.132	1.00	14.91
ATOM	363	N	ALA	46	-.606	12.682	-4.441	1.00	14.60
ATOM	364	CA	ALA	46	-1.928	12.172	-4.821	1.00	14.34
ATOM	365	CB	ALA	46	-2.674	13.203	-5.648	1.00	14.80
ATOM	366	C	ALA	46	-1.787	10.864	-5.610	1.00	15.20
ATOM	367	O	ALA	46	-2.551	9.918	-5.411	1.00	15.04
ATOM	368	N	GLN	47	-.805	10.823	-6.515	1.00	15.56
ATOM	369	CA	GLN	47	-.544	9.630	-7.314	1.00	16.17
ATOM	370	CB	GLN	47	.570	9.915	-8.331	1.00	18.77
ATOM	371	CG	GLN	47	.271	11.135	-9.194	1.00	22.49
ATOM	372	CD	GLN	47	1.169	11.276	-10.413	1.00	25.42
ATOM	373	OE1	GLN	47	2.370	10.952	-10.389	1.00	27.30

ATOM	374	NE2	GLN	47	.592	11.791	-11.492	1.00	27.37
ATOM	375	C	GLN	47	-.140	8.471	-6.402	1.00	15.04
ATOM	376	O	GLN	47	-.566	7.327	-6.587	1.00	15.71
ATOM	377	N	VAL	48	.684	8.765	-5.410	1.00	14.34
ATOM	378	CA	VAL	48	1.117	7.725	-4.495	1.00	13.08
ATOM	379	CB	VAL	48	2.159	8.257	-3.508	1.00	13.45
ATOM	380	CG1	VAL	48	2.489	7.180	-2.475	1.00	13.68
ATOM	381	CG2	VAL	48	3.421	8.656	-4.272	1.00	13.57
ATOM	382	C	VAL	48	-.070	7.125	-3.737	1.00	12.42
ATOM	383	O	VAL	48	-.252	5.908	-3.709	1.00	13.11
ATOM	384	N	ILE	49	-.894	7.981	-3.141	1.00	12.10
ATOM	385	CA	ILE	49	-2.058	7.509	-2.391	1.00	11.49
ATOM	386	CB	ILE	49	-2.798	8.698	-1.719	1.00	9.68
ATOM	387	CG2	ILE	49	-4.045	8.198	-.977	1.00	10.69
ATOM	388	CG1	ILE	49	-1.846	9.419	-.755	1.00	10.21
ATOM	389	CD1	ILE	49	-2.384	10.727	-.181	1.00	9.57
ATOM	390	C	ILE	49	-3.035	6.732	-3.278	1.00	11.74
ATOM	391	O	ILE	49	-3.550	5.685	-2.880	1.00	11.40
ATOM	392	N	ALA	50	-3.275	7.234	-4.488	1.00	12.60
ATOM	393	CA	ALA	50	-4.200	6.592	-5.409	1.00	12.63
ATOM	394	CB	ALA	50	-4.378	7.463	-6.649	1.00	13.17
ATOM	395	C	ALA	50	-3.740	5.195	-5.824	1.00	12.65
ATOM	396	O	ALA	50	-4.559	4.328	-6.127	1.00	13.18
ATOM	397	N	SER	51	-2.428	4.976	-5.834	1.00	12.83
ATOM	398	CA	SER	51	-1.906	3.681	-6.248	1.00	12.99
ATOM	399	CB	SER	51	-.399	3.775	-6.495	1.00	12.13
ATOM	400	OG	SER	51	.333	3.896	-5.295	1.00	13.36
ATOM	401	C	SER	51	-2.227	2.543	-5.279	1.00	12.63
ATOM	402	O	SER	51	-2.072	1.381	-5.621	1.00	13.66
ATOM	403	N	TYR	52	-2.675	2.868	-4.068	1.00	12.00
ATOM	404	CA	TYR	52	-3.033	1.836	-3.102	1.00	11.24
ATOM	405	CB	TYR	52	-3.039	2.406	-1.678	1.00	10.27
ATOM	406	CG	TYR	52	-1.651	2.601	-1.105	1.00	10.00
ATOM	407	CD1	TYR	52	-.895	3.728	-1.422	1.00	10.00
ATOM	408	CE1	TYR	52	.385	3.905	-.914	1.00	9.14
ATOM	409	CD2	TYR	52	-1.085	1.643	-.260	1.00	9.84
ATOM	410	CE2	TYR	52	.200	1.811	.251	1.00	8.93
ATOM	411	CZ	TYR	52	.926	2.955	-.083	1.00	9.17
ATOM	412	OH	TYR	52	2.184	3.150	.442	1.00	10.25
ATOM	413	C	TYR	52	-4.424	1.317	-3.440	1.00	12.03
ATOM	414	O	TYR	52	-4.899	.340	-2.856	1.00	12.38
ATOM	415	N	GLY	53	-5.079	1.985	-4.383	1.00	12.39
ATOM	416	CA	GLY	53	-6.413	1.566	-4.765	1.00	13.57
ATOM	417	C	GLY	53	-7.367	1.477	-3.592	1.00	13.86
ATOM	418	O	GLY	53	-7.362	2.342	-2.702	1.00	14.23
ATOM	419	N	SER	54	-8.173	.420	-3.580	1.00	14.22
ATOM	420	CA	SER	54	-9.184	.228	-2.541	1.00	14.51
ATOM	421	CB	SER	54	-10.180	-.847	-2.984	1.00	15.25
ATOM	422	OG	SER	54	-9.550	-2.113	-3.023	1.00	17.12
ATOM	423	C	SER	54	-8.656	-.110	-1.142	1.00	13.94
ATOM	424	O	SER	54	-9.429	-.232	-.188	1.00	13.93
ATOM	425	N	ALA	55	-7.345	-.251	-.996	1.00	13.88
ATOM	426	CA	ALA	55	-6.801	-.559	.317	1.00	12.98
ATOM	427	CB	ALA	55	-5.310	-.818	.217	1.00	13.06
ATOM	428	C	ALA	55	-7.096	.609	1.268	1.00	12.53
ATOM	429	O	ALA	55	-7.163	.423	2.486	1.00	11.81
ATOM	430	N	VAL	56	-7.299	1.799	.706	1.00	11.88
ATOM	431	CA	VAL	56	-7.617	2.987	1.498	1.00	11.69
ATOM	432	CB	VAL	56	-6.390	3.899	1.710	1.00	12.31
ATOM	433	CG1	VAL	56	-5.262	3.144	2.417	1.00	11.57

ATOM	434	CG2	VAL	56	-5.934	4.451	.368	1.00	13.82
ATOM	435	C	VAL	56	-8.644	3.812	.739	1.00	12.44
ATOM	436	O	VAL	56	-8.935	3.520	-.419	1.00	13.14
ATOM	437	N	THR	57	-9.213	4.811	1.411	1.00	11.55
ATOM	438	CA	THR	57	-10.154	5.730	.785	1.00	12.51
ATOM	439	CB	THR	57	-11.475	5.900	1.575	1.00	12.87
ATOM	440	OG1	THR	57	-12.150	4.644	1.678	1.00	13.84
ATOM	441	CG2	THR	57	-12.394	6.886	.843	1.00	13.67
ATOM	442	C	THR	57	-9.413	7.066	.790	1.00	12.09
ATOM	443	O	THR	57	-9.020	7.574	1.843	1.00	12.96
ATOM	444	N	HIS	58	-9.257	7.648	-.390	1.00	11.15
ATOM	445	CA	HIS	58	-8.540	8.899	-.561	1.00	10.89
ATOM	446	CB	HIS	58	-7.665	8.749	-1.811	1.00	10.68
ATOM	447	CG	HIS	58	-6.800	9.928	-2.118	1.00	11.33
ATOM	448	CD2	HIS	58	-6.421	10.987	-1.364	1.00	12.01
ATOM	449	ND1	HIS	58	-6.182	10.085	-3.343	1.00	12.61
ATOM	450	CE1	HIS	58	-5.461	11.193	-3.329	1.00	13.26
ATOM	451	NE2	HIS	58	-5.589	11.758	-2.140	1.00	12.53
ATOM	452	C	HIS	58	-9.512	10.071	-.706	1.00	11.13
ATOM	453	O	HIS	58	-10.327	10.081	-1.632	1.00	11.72
ATOM	454	N	ILE	59	-9.462	11.034	.218	1.00	9.54
ATOM	455	CA	ILE	59	-10.333	12.207	.124	1.00	10.23
ATOM	456	CB	ILE	59	-11.329	12.334	1.330	1.00	9.70
ATOM	457	CG2	ILE	59	-12.215	11.072	1.412	1.00	10.92
ATOM	458	CG1	ILE	59	-10.581	12.507	2.654	1.00	9.57
ATOM	459	CD1	ILE	59	-11.518	12.643	3.870	1.00	10.73
ATOM	460	C	ILE	59	-9.426	13.421	.043	1.00	10.33
ATOM	461	O	ILE	59	-8.290	13.385	.524	1.00	10.28
ATOM	462	N	ARG	60	-9.923	14.501	-.545	1.00	11.08
ATOM	463	CA	ARG	60	-9.102	15.692	-.741	1.00	12.46
ATOM	464	CB	ARG	60	-8.845	15.857	-2.243	1.00	14.43
ATOM	465	CG	ARG	60	-8.267	14.603	-2.926	1.00	18.13
ATOM	466	CD	ARG	60	-8.259	14.743	-4.466	1.00	22.27
ATOM	467	NE	ARG	60	-7.549	13.642	-5.129	1.00	25.41
ATOM	468	CZ	ARG	60	-6.872	13.751	-6.275	1.00	26.68
ATOM	469	NH1	ARG	60	-6.799	14.919	-6.915	1.00	27.81
ATOM	470	NH2	ARG	60	-6.252	12.690	-6.785	1.00	27.23
ATOM	471	C	ARG	60	-9.704	16.974	-.182	1.00	11.97
ATOM	472	O	ARG	60	-10.811	17.365	-.556	1.00	13.18
ATOM	473	N	GLN	61	-8.984	17.616	.730	1.00	11.64
ATOM	474	CA	GLN	61	-9.448	18.870	1.314	1.00	11.40
ATOM	475	CB	GLN	61	-8.394	19.384	2.308	1.00	11.68
ATOM	476	CG	GLN	61	-8.923	20.414	3.293	1.00	10.95
ATOM	477	CD	GLN	61	-9.105	21.796	2.678	1.00	10.83
ATOM	478	OE1	GLN	61	-10.226	22.315	2.601	1.00	11.60
ATOM	479	NE2	GLN	61	-8.001	22.409	2.259	1.00	10.29
ATOM	480	C	GLN	61	-9.662	19.826	.118	1.00	12.30
ATOM	481	O	GLN	61	-8.729	20.148	-.599	1.00	12.45
ATOM	482	N	PRO	62	-10.909	20.285	-.096	1.00	13.42
ATOM	483	CD	PRO	62	-12.008	20.026	.855	1.00	12.77
ATOM	484	CA	PRO	62	-11.374	21.176	-1.172	1.00	13.77
ATOM	485	CB	PRO	62	-12.884	21.111	-1.019	1.00	13.22
ATOM	486	CG	PRO	62	-13.036	21.082	.469	1.00	14.21
ATOM	487	C	PRO	62	-10.907	22.625	-1.287	1.00	14.06
ATOM	488	O	PRO	62	-10.814	23.158	-2.396	1.00	15.11
ATOM	489	N	ASP	63	-10.648	23.279	-.169	1.00	14.23
ATOM	490	CA	ASP	63	-10.260	24.682	-.206	1.00	15.53
ATOM	491	CB	ASP	63	-10.955	25.416	.927	1.00	16.62
ATOM	492	CG	ASP	63	-11.031	26.896	.693	1.00	18.66
ATOM	493	OD1	ASP	63	-10.148	27.432	-.023	1.00	18.69

ATOM	494	OD2	ASP	63	-11.972	27.512	1.245	1.00	19.61
ATOM	495	C	ASP	63	-8.765	24.918	-.107	1.00	15.51
ATOM	496	O	ASP	63	-8.226	24.968	.994	1.00	15.35
ATOM	497	N	LEU	64	-8.106	25.093	-1.250	1.00	15.86
ATOM	498	CA	LEU	64	-6.665	25.309	-1.262	1.00	15.89
ATOM	499	CB	LEU	64	-6.039	24.579	-2.457	1.00	17.02
ATOM	500	CG	LEU	64	-6.391	23.087	-2.576	1.00	18.13
ATOM	501	CD1	LEU	64	-5.634	22.496	-3.751	1.00	19.11
ATOM	502	CD2	LEU	64	-6.067	22.339	-1.257	1.00	19.70
ATOM	503	C	LEU	64	-6.238	26.779	-1.242	1.00	16.22
ATOM	504	O	LEU	64	-5.052	27.090	-1.400	1.00	17.15
ATOM	505	N	SER	65	-7.178	27.682	-.995	1.00	15.51
ATOM	506	CA	SER	65	-6.843	29.101	-.974	1.00	16.02
ATOM	507	CB	SER	65	-8.114	29.934	-1.011	1.00	15.88
ATOM	508	OG	SER	65	-8.811	29.787	.209	1.00	16.92
ATOM	509	C	SER	65	-6.035	29.520	.245	1.00	16.96
ATOM	510	O	SER	65	-5.916	28.782	1.225	1.00	16.34
ATOM	511	N	ASN	66	-5.500	30.732	.184	1.00	17.05
ATOM	512	CA	ASN	66	-4.724	31.285	1.284	1.00	18.00
ATOM	513	CB	ASN	66	-3.845	32.422	.788	1.00	20.78
ATOM	514	CG	ASN	66	-2.438	31.977	.566	1.00	23.43
ATOM	515	OD1	ASN	66	-2.199	30.906	-.007	1.00	25.92
ATOM	516	ND2	ASN	66	-1.482	32.781	1.031	1.00	26.27
ATOM	517	C	ASN	66	-5.661	31.794	2.356	1.00	17.26
ATOM	518	O	ASN	66	-6.753	32.263	2.067	1.00	17.54
ATOM	519	N	ILE	67	-5.220	31.701	3.602	1.00	16.21
ATOM	520	CA	ILE	67	-6.034	32.117	4.727	1.00	16.30
ATOM	521	CB	ILE	67	-5.980	31.037	5.844	1.00	15.16
ATOM	522	CG2	ILE	67	-6.734	31.501	7.076	1.00	15.41
ATOM	523	CG1	ILE	67	-6.586	29.732	5.313	1.00	14.89
ATOM	524	CD1	ILE	67	-6.083	28.490	6.013	1.00	15.28
ATOM	525	C	ILE	67	-5.555	33.453	5.272	1.00	16.40
ATOM	526	O	ILE	67	-4.352	33.686	5.388	1.00	17.27
ATOM	527	N	ALA	68	-6.504	34.336	5.571	1.00	16.23
ATOM	528	CA	ALA	68	-6.188	35.636	6.143	1.00	16.26
ATOM	529	CB	ALA	68	-7.413	36.526	6.109	1.00	16.44
ATOM	530	C	ALA	68	-5.770	35.368	7.593	1.00	15.15
ATOM	531	O	ALA	68	-6.550	34.789	8.377	1.00	16.64
ATOM	532	N	VAL	69	-4.544	35.751	7.946	1.00	14.20
ATOM	533	CA	VAL	69	-4.038	35.536	9.308	1.00	12.68
ATOM	534	CB	VAL	69	-2.557	35.037	9.298	1.00	11.83
ATOM	535	CG1	VAL	69	-2.422	33.812	8.390	1.00	12.71
ATOM	536	CG2	VAL	69	-1.624	36.134	8.815	1.00	12.62
ATOM	537	C	VAL	69	-4.133	36.815	10.139	1.00	12.30
ATOM	538	O	VAL	69	-4.309	37.901	9.595	1.00	12.60
ATOM	539	N	GLN	70	-4.041	36.687	11.460	1.00	11.86
ATOM	540	CA	GLN	70	-4.109	37.860	12.331	1.00	11.72
ATOM	541	CB	GLN	70	-4.523	37.456	13.752	1.00	12.37
ATOM	542	CG	GLN	70	-6.022	37.149	13.867	1.00	13.86
ATOM	543	CD	GLN	70	-6.898	38.357	13.577	1.00	15.84
ATOM	544	OE1	GLN	70	-7.643	38.395	12.572	1.00	19.43
ATOM	545	NE2	GLN	70	-6.826	39.355	14.456	1.00	13.96
ATOM	546	C	GLN	70	-2.757	38.569	12.306	1.00	11.06
ATOM	547	O	GLN	70	-1.762	37.981	11.893	1.00	10.50
ATOM	548	N	PRO	71	-2.697	39.831	12.775	1.00	11.30
ATOM	549	CD	PRO	71	-3.772	40.596	13.430	1.00	10.91
ATOM	550	CA	PRO	71	-1.443	40.599	12.762	1.00	10.57
ATOM	551	CB	PRO	71	-1.840	41.942	13.378	1.00	11.12
ATOM	552	CG	PRO	71	-3.325	42.003	13.203	1.00	10.87
ATOM	553	C	PRO	71	-.204	40.032	13.431	1.00	11.20

ATOM	554	O	PRO	71	.916	40.469	13.129	1.00	12.30
ATOM	555	N	ASP	72	-.385	39.093	14.354	1.00	10.60
ATOM	556	CA	ASP	72	.758	38.518	15.049	1.00	10.55
ATOM	557	CB	ASP	72	.390	38.229	16.528	1.00	10.40
ATOM	558	CG	ASP	72	-.878	37.377	16.691	1.00	10.31
ATOM	559	OD1	ASP	72	-1.767	37.427	15.811	1.00	9.34
ATOM	560	OD2	ASP	72	-1.000	36.659	17.720	1.00	10.23
ATOM	561	C	ASP	72	1.247	37.239	14.378	1.00	10.45
ATOM	562	O	ASP	72	2.226	36.640	14.821	1.00	10.60
ATOM	563	N	HIS	73	.611	36.864	13.271	1.00	11.08
ATOM	564	CA	HIS	73	.922	35.581	12.646	1.00	11.21
ATOM	565	CB	HIS	73	-.307	34.681	12.778	1.00	10.93
ATOM	566	CG	HIS	73	-.654	34.312	14.184	1.00	10.68
ATOM	567	CD2	HIS	73	.115	34.172	15.288	1.00	8.85
ATOM	568	ND1	HIS	73	-1.931	33.946	14.555	1.00	9.89
ATOM	569	CE1	HIS	73	-1.929	33.590	15.827	1.00	10.53
ATOM	570	NE2	HIS	73	-.701	33.717	16.296	1.00	10.14
ATOM	571	C	HIS	73	1.387	35.533	11.194	1.00	12.23
ATOM	572	O	HIS	73	1.181	34.518	10.523	1.00	11.51
ATOM	573	N	ARG	74	2.015	36.592	10.699	1.00	13.47
ATOM	574	CA	ARG	74	2.457	36.565	9.313	1.00	15.55
ATOM	575	CB	ARG	74	3.152	37.887	8.946	1.00	17.41
ATOM	576	CG	ARG	74	2.194	38.947	8.379	1.00	21.51
ATOM	577	CD	ARG	74	1.717	40.002	9.408	1.00	24.64
ATOM	578	NE	ARG	74	.525	40.696	8.894	1.00	27.02
ATOM	579	CZ	ARG	74	-.014	41.804	9.408	1.00	27.80
ATOM	580	NH1	ARG	74	.503	42.407	10.475	1.00	28.09
ATOM	581	NH2	ARG	74	-1.087	42.322	8.833	1.00	29.04
ATOM	582	C	ARG	74	3.361	35.380	8.974	1.00	15.70
ATOM	583	O	ARG	74	3.318	34.865	7.843	1.00	16.60
ATOM	584	N	LYS	75	4.169	34.936	9.934	1.00	15.09
ATOM	585	CA	LYS	75	5.079	33.809	9.712	1.00	15.77
ATOM	586	CB	LYS	75	6.178	33.757	10.793	1.00	17.31
ATOM	587	CG	LYS	75	7.123	34.932	10.941	1.00	19.63
ATOM	588	CD	LYS	75	7.956	34.695	12.200	1.00	20.96
ATOM	589	CE	LYS	75	9.327	35.319	12.110	1.00	22.44
ATOM	590	NZ	LYS	75	10.141	34.976	13.307	1.00	22.23
ATOM	591	C	LYS	75	4.362	32.461	9.799	1.00	15.99
ATOM	592	O	LYS	75	4.944	31.438	9.439	1.00	16.81
ATOM	593	N	PHE	76	3.112	32.448	10.265	1.00	14.16
ATOM	594	CA	PHE	76	2.416	31.181	10.498	1.00	14.36
ATOM	595	CB	PHE	76	2.008	31.173	11.977	1.00	14.08
ATOM	596	CG	PHE	76	3.151	31.500	12.901	1.00	14.70
ATOM	597	CD1	PHE	76	3.205	32.708	13.602	1.00	14.55
ATOM	598	CD2	PHE	76	4.225	30.615	13.018	1.00	15.29
ATOM	599	CE1	PHE	76	4.326	33.019	14.403	1.00	15.53
ATOM	600	CE2	PHE	76	5.339	30.912	13.809	1.00	15.96
ATOM	601	CZ	PHE	76	5.395	32.116	14.505	1.00	15.31
ATOM	602	C	PHE	76	1.258	30.694	9.612	1.00	14.56
ATOM	603	O	PHE	76	.401	29.935	10.079	1.00	13.83
ATOM	604	N	GLN	77	1.254	31.083	8.336	1.00	15.42
ATOM	605	CA	GLN	77	-.214	30.648	7.389	1.00	16.00
ATOM	606	CB	GLN	77	.595	31.035	5.950	1.00	17.39
ATOM	607	CG	GLN	77	-.319	30.436	4.866	1.00	20.36
ATOM	608	CD	GLN	77	-1.719	31.013	4.901	1.00	21.37
ATOM	609	OE1	GLN	77	-2.674	30.438	4.341	1.00	22.63
ATOM	610	NE2	GLN	77	-1.857	32.157	5.549	1.00	21.20
ATOM	611	C	GLN	77	.033	29.118	7.449	1.00	15.38
ATOM	612	O	GLN	77	-1.090	28.614	7.471	1.00	14.64
ATOM	613	N	GLY	78	1.146	28.389	7.487	1.00	14.34

ATOM	614	CA	GLY	78	1.090	26.934	7.527	1.00	13.86
ATOM	615	C	GLY	78	.295	26.341	8.682	1.00	13.01
ATOM	616	O	GLY	78	-.345	25.290	8.527	1.00	13.45
ATOM	617	N	TYR	79	.331	26.993	9.845	1.00	12.03
ATOM	618	CA	TYR	79	-.408	26.495	11.005	1.00	12.20
ATOM	619	CB	TYR	79	.097	27.146	12.283	1.00	13.01
ATOM	620	CG	TYR	79	1.419	26.588	12.699	1.00	16.21
ATOM	621	CD1	TYR	79	2.609	27.166	12.267	1.00	17.14
ATOM	622	CE1	TYR	79	3.841	26.647	12.658	1.00	19.14
ATOM	623	CD2	TYR	79	1.486	25.465	13.530	1.00	17.32
ATOM	624	CE2	TYR	79	2.720	24.932	13.928	1.00	19.52
ATOM	625	CZ	TYR	79	3.893	25.534	13.491	1.00	20.08
ATOM	626	OH	TYR	79	5.126	25.049	13.906	1.00	22.39
ATOM	627	C	TYR	79	-1.896	26.720	10.861	1.00	11.35
ATOM	628	O	TYR	79	-2.695	25.962	11.421	1.00	11.37
ATOM	629	N	TYR	80	-2.268	27.777	10.136	1.00	10.62
ATOM	630	CA	TYR	80	-3.666	28.077	9.868	1.00	9.57
ATOM	631	CB	TYR	80	-3.810	29.467	9.218	1.00	9.87
ATOM	632	CG	TYR	80	-3.853	30.630	10.186	1.00	9.40
ATOM	633	CD1	TYR	80	-2.711	31.033	10.873	1.00	9.76
ATOM	634	CE1	TYR	80	-2.740	32.126	11.738	1.00	9.60
ATOM	635	CD2	TYR	80	-5.028	31.344	10.390	1.00	8.56
ATOM	636	CE2	TYR	80	-5.067	32.453	11.259	1.00	9.17
ATOM	637	CZ	TYR	80	-3.918	32.827	11.920	1.00	9.35
ATOM	638	OH	TYR	80	-3.933	33.911	12.759	1.00	9.62
ATOM	639	C	TYR	80	-4.199	27.014	8.896	1.00	9.45
ATOM	640	O	TYR	80	-5.344	26.559	9.001	1.00	10.80
ATOM	641	N	LYS	81	-3.380	26.630	7.922	1.00	10.11
ATOM	642	CA	LYS	81	-3.816	25.611	6.974	1.00	10.68
ATOM	643	CB	LYS	81	-2.841	25.517	5.806	1.00	12.12
ATOM	644	CG	LYS	81	-2.846	26.797	4.979	1.00	15.10
ATOM	645	CD	LYS	81	-2.118	26.632	3.673	1.00	17.28
ATOM	646	CE	LYS	81	-2.213	27.904	2.832	1.00	19.39
ATOM	647	NZ	LYS	81	-1.820	27.601	1.449	1.00	21.54
ATOM	648	C	LYS	81	-3.981	24.257	7.650	1.00	10.21
ATOM	649	O	LYS	81	-4.933	23.544	7.367	1.00	9.93
ATOM	650	N	ILE	82	-3.056	23.910	8.546	1.00	9.96
ATOM	651	CA	ILE	82	-3.138	22.642	9.267	1.00	9.92
ATOM	652	CB	ILE	82	-1.914	22.456	10.218	1.00	10.95
ATOM	653	CG2	ILE	82	-2.119	21.241	11.111	1.00	11.76
ATOM	654	CG1	ILE	82	-.639	22.246	9.390	1.00	11.33
ATOM	655	CD1	ILE	82	.641	22.184	10.203	1.00	12.88
ATOM	656	C	ILE	82	-4.448	22.601	10.067	1.00	9.70
ATOM	657	O	ILE	82	-5.163	21.589	10.058	1.00	9.49
ATOM	658	N	ALA	83	-4.779	23.700	10.748	1.00	9.64
ATOM	659	CA	ALA	83	-6.020	23.733	11.525	1.00	8.25
ATOM	660	CB	ALA	83	-6.114	25.025	12.336	1.00	9.69
ATOM	661	C	ALA	83	-7.231	23.585	10.619	1.00	8.44
ATOM	662	O	ALA	83	-8.181	22.884	10.959	1.00	8.16
ATOM	663	N	ARG	84	-7.212	24.249	9.467	1.00	7.93
ATOM	664	CA	ARG	84	-8.330	24.120	8.531	1.00	8.42
ATOM	665	CB	ARG	84	-8.126	25.035	7.306	1.00	9.93
ATOM	666	CG	ARG	84	-9.148	24.771	6.179	1.00	10.35
ATOM	667	CD	ARG	84	-9.021	25.758	5.012	1.00	11.07
ATOM	668	NE	ARG	84	-7.736	25.640	4.327	1.00	11.85
ATOM	669	CZ	ARG	84	-7.313	26.487	3.393	1.00	12.22
ATOM	670	NH1	ARG	84	-8.076	27.514	3.035	1.00	12.06
ATOM	671	NH2	ARG	84	-6.134	26.306	2.818	1.00	13.30
ATOM	672	C	ARG	84	-8.455	22.659	8.067	1.00	8.72
ATOM	673	O	ARG	84	-9.554	22.117	8.003	1.00	9.22

ATOM	674	N	HIS	85	-7.331	22.026	7.742	1.00	8.53
ATOM	675	CA	HIS	85	-7.354	20.634	7.277	1.00	7.80
ATOM	676	CB	HIS	85	-5.941	20.152	6.895	1.00	7.69
ATOM	677	CG	HIS	85	-5.925	18.800	6.239	1.00	7.19
ATOM	678	CD2	HIS	85	-6.920	18.072	5.679	1.00	8.31
ATOM	679	ND1	HIS	85	-4.779	18.043	6.107	1.00	8.38
ATOM	680	CE1	HIS	85	-5.072	16.906	5.499	1.00	8.26
ATOM	681	NE2	HIS	85	-6.364	16.901	5.226	1.00	8.27
ATOM	682	C	HIS	85	-7.944	19.695	8.324	1.00	8.54
ATOM	683	O	HIS	85	-8.806	18.876	8.014	1.00	7.88
ATOM	684	N	TYR	86	-7.486	19.821	9.563	1.00	8.60
ATOM	685	CA	TYR	86	-8.006	18.981	10.647	1.00	9.23
ATOM	686	CB	TYR	86	-7.317	19.334	11.969	1.00	9.31
ATOM	687	CG	TYR	86	-6.095	18.496	12.246	1.00	9.75
ATOM	688	CD1	TYR	86	-4.918	18.662	11.514	1.00	10.10
ATOM	689	CE1	TYR	86	-3.808	17.858	11.749	1.00	10.25
ATOM	690	CD2	TYR	86	-6.126	17.498	13.225	1.00	10.54
ATOM	691	CE2	TYR	86	-5.020	16.685	13.458	1.00	11.11
ATOM	692	CZ	TYR	86	-3.867	16.865	12.723	1.00	10.89
ATOM	693	OH	TYR	86	-2.776	16.064	12.958	1.00	10.18
ATOM	694	C	TYR	86	-9.516	19.161	10.791	1.00	10.12
ATOM	695	O	TYR	86	-10.250	18.185	10.929	1.00	9.53
ATOM	696	N	ARG	87	-9.977	20.410	10.769	1.00	10.28
ATOM	697	CA	ARG	87	-11.399	20.698	10.891	1.00	11.82
ATOM	698	CB	ARG	87	-11.635	22.205	10.791	1.00	14.45
ATOM	699	CG	ARG	87	-13.059	22.637	11.079	1.00	19.04
ATOM	700	CD	ARG	87	-13.237	24.100	10.750	1.00	22.77
ATOM	701	NE	ARG	87	-14.576	24.544	11.121	1.00	28.03
ATOM	702	CZ	ARG	87	-15.064	25.770	10.921	1.00	29.41
ATOM	703	NH1	ARG	87	-14.323	26.716	10.335	1.00	30.95
ATOM	704	NH2	ARG	87	-16.306	26.054	11.313	1.00	31.09
ATOM	705	C	ARG	87	-12.181	19.984	9.794	1.00	11.17
ATOM	706	O	ARG	87	-13.227	19.363	10.050	1.00	12.29
ATOM	707	N	TRP	88	-11.676	20.062	8.565	1.00	9.72
ATOM	708	CA	TRP	88	-12.355	19.419	7.447	1.00	9.55
ATOM	709	CB	TRP	88	-11.783	19.908	6.108	1.00	8.96
ATOM	710	CG	TRP	88	-12.510	19.340	4.920	1.00	9.06
ATOM	711	CD2	TRP	88	-12.149	18.171	4.172	1.00	9.56
ATOM	712	CE2	TRP	88	-13.135	17.988	3.169	1.00	10.05
ATOM	713	CE3	TRP	88	-11.086	17.258	4.249	1.00	9.28
ATOM	714	CD1	TRP	88	-13.670	19.807	4.357	1.00	10.02
ATOM	715	NE1	TRP	88	-14.048	18.998	3.302	1.00	9.74
ATOM	716	CZ2	TRP	88	-13.088	16.926	2.251	1.00	10.81
ATOM	717	CZ3	TRP	88	-11.042	16.201	3.334	1.00	10.21
ATOM	718	CH2	TRP	88	-12.036	16.046	2.351	1.00	9.99
ATOM	719	C	TRP	88	-12.294	17.898	7.480	1.00	9.92
ATOM	720	O	TRP	88	-13.301	17.232	7.281	1.00	9.80
ATOM	721	N	ALA	89	-11.110	17.346	7.715	1.00	9.69
ATOM	722	CA	ALA	89	-10.960	15.897	7.746	1.00	9.55
ATOM	723	CB	ALA	89	-9.482	15.521	7.850	1.00	9.44
ATOM	724	C	ALA	89	-11.747	15.261	8.877	1.00	9.09
ATOM	725	O	ALA	89	-12.363	14.220	8.687	1.00	9.88
ATOM	726	N	LEU	90	-11.724	15.858	10.061	1.00	9.60
ATOM	727	CA	LEU	90	-12.480	15.287	11.169	1.00	9.21
ATOM	728	CB	LEU	90	-12.124	15.989	12.476	1.00	10.41
ATOM	729	CG	LEU	90	-10.746	15.666	13.050	1.00	10.71
ATOM	730	CD1	LEU	90	-10.392	16.697	14.132	1.00	12.61
ATOM	731	CD2	LEU	90	-10.743	14.239	13.608	1.00	12.38
ATOM	732	C	LEU	90	-13.970	15.417	10.881	1.00	9.86
ATOM	733	O	LEU	90	-14.755	14.543	11.232	1.00	9.76

ATOM	734	N	GLY	91	-14.356	16.503	10.220	1.00	9.81
ATOM	735	CA	GLY	91	-15.763	16.683	9.882	1.00	10.54
ATOM	736	C	GLY	91	-16.165	15.563	8.941	1.00	10.12
ATOM	737	O	GLY	91	-17.268	15.033	9.010	1.00	10.68
ATOM	738	N	GLN	92	-15.268	15.185	8.039	1.00	10.67
ATOM	739	CA	GLN	92	-15.592	14.108	7.096	1.00	11.25
ATOM	740	CB	GLN	92	-14.502	13.993	6.016	1.00	12.48
ATOM	741	CG	GLN	92	-14.507	15.159	5.038	1.00	14.80
ATOM	742	CD	GLN	92	-15.755	15.159	4.166	1.00	17.43
ATOM	743	OE1	GLN	92	-15.983	14.217	3.394	1.00	19.55
ATOM	744	NE2	GLN	92	-16.574	16.201	4.287	1.00	19.05
ATOM	745	C	GLN	92	-15.775	12.756	7.775	1.00	12.04
ATOM	746	O	GLN	92	-16.741	12.027	7.510	1.00	11.70
ATOM	747	N	ILE	93	-14.859	12.416	8.670	1.00	10.84
ATOM	748	CA	ILE	93	-14.952	11.126	9.330	1.00	11.21
ATOM	749	CB	ILE	93	-13.658	10.799	10.152	1.00	13.37
ATOM	750	CG2	ILE	93	-12.431	11.102	9.324	1.00	15.10
ATOM	751	CG1	ILE	93	-13.607	11.586	11.451	1.00	15.36
ATOM	752	CD1	ILE	93	-12.404	11.242	12.272	1.00	19.12
ATOM	753	C	ILE	93	-16.176	11.005	10.228	1.00	11.68
ATOM	754	O	ILE	93	-16.797	9.942	10.312	1.00	11.42
ATOM	755	N	PHE	94	-16.552	12.101	10.873	1.00	11.11
ATOM	756	CA	PHE	94	-17.673	12.051	11.803	1.00	12.36
ATOM	757	CB	PHE	94	-17.341	12.919	13.027	1.00	12.02
ATOM	758	CG	PHE	94	-16.242	12.346	13.886	1.00	11.07
ATOM	759	CD1	PHE	94	-15.123	13.105	14.215	1.00	10.61
ATOM	760	CD2	PHE	94	-16.317	11.034	14.344	1.00	10.99
ATOM	761	CE1	PHE	94	-14.089	12.555	14.989	1.00	9.27
ATOM	762	CE2	PHE	94	-15.304	10.484	15.106	1.00	10.05
ATOM	763	CZ	PHE	94	-14.180	11.241	15.431	1.00	10.31
ATOM	764	C	PHE	94	-19.037	12.401	11.239	1.00	14.44
ATOM	765	O	PHE	94	-20.055	11.885	11.709	1.00	15.45
ATOM	766	N	HIS	95	-19.064	13.271	10.239	1.00	15.44
ATOM	767	CA	HIS	95	-20.322	13.667	9.622	1.00	17.02
ATOM	768	CB	HIS	95	-20.319	15.162	9.291	1.00	17.83
ATOM	769	CG	HIS	95	-20.209	16.036	10.497	1.00	20.46
ATOM	770	CD2	HIS	95	-19.432	17.114	10.755	1.00	20.92
ATOM	771	ND1	HIS	95	-20.915	15.786	11.654	1.00	21.51
ATOM	772	CE1	HIS	95	-20.570	16.669	12.575	1.00	22.03
ATOM	773	NE2	HIS	95	-19.672	17.485	12.055	1.00	21.61
ATOM	774	C	HIS	95	-20.592	12.860	8.372	1.00	17.29
ATOM	775	O	HIS	95	-21.562	12.127	8.306	1.00	18.73
ATOM	776	N	ASN	96	-19.720	12.956	7.383	1.00	16.80
ATOM	777	CA	ASN	96	-19.962	12.228	6.151	1.00	16.96
ATOM	778	CB	ASN	96	-19.022	12.742	5.065	1.00	18.84
ATOM	779	CG	ASN	96	-19.182	14.240	4.832	1.00	21.26
ATOM	780	OD1	ASN	96	-19.598	14.681	3.747	1.00	23.78
ATOM	781	ND2	ASN	96	-18.875	15.039	5.858	1.00	22.06
ATOM	782	C	ASN	96	-19.871	10.720	6.295	1.00	16.77
ATOM	783	O	ASN	96	-20.812	10.011	5.916	1.00	16.82
ATOM	784	N	PHE	97	-18.768	10.211	6.840	1.00	15.16
ATOM	785	CA	PHE	97	-18.632	8.761	6.990	1.00	15.02
ATOM	786	CB	PHE	97	-17.154	8.345	7.108	1.00	15.55
ATOM	787	CG	PHE	97	-16.347	8.516	5.838	1.00	16.52
ATOM	788	CD1	PHE	97	-15.774	9.742	5.515	1.00	17.42
ATOM	789	CD2	PHE	97	-16.117	7.430	4.989	1.00	17.55
ATOM	790	CE1	PHE	97	-14.984	9.886	4.367	1.00	17.54
ATOM	791	CE2	PHE	97	-15.330	7.564	3.844	1.00	17.59
ATOM	792	CZ	PHE	97	-14.765	8.794	3.532	1.00	17.80
ATOM	793	C	PHE	97	-19.409	8.244	8.209	1.00	15.04

ATOM	794	O	PHE	97	-19.665	7.043	8.337	1.00	15.85
ATOM	795	N	ASN	98	-19.754	9.161	9.112	1.00	14.18
ATOM	796	CA	ASN	98	-20.512	8.864	10.330	1.00	14.87
ATOM	797	CB	ASN	98	-21.962	8.501	9.958	1.00	16.80
ATOM	798	CG	ASN	98	-22.870	8.376	11.174	1.00	18.89
ATOM	799	OD1	ASN	98	-23.603	7.391	11.301	1.00	21.71
ATOM	800	ND2	ASN	98	-22.837	9.368	12.071	1.00	20.84
ATOM	801	C	ASN	98	-19.915	7.773	11.238	1.00	13.85
ATOM	802	O	ASN	98	-20.636	6.940	11.785	1.00	14.42
ATOM	803	N	TYR	99	-18.591	7.797	11.418	1.00	12.63
ATOM	804	CA	TYR	99	-17.919	6.837	12.291	1.00	11.79
ATOM	805	CB	TYR	99	-16.438	6.734	11.935	1.00	11.03
ATOM	806	CG	TYR	99	-16.173	5.970	10.674	1.00	11.77
ATOM	807	CD1	TYR	99	-15.568	6.580	9.576	1.00	12.08
ATOM	808	CE1	TYR	99	-15.276	5.851	8.413	1.00	13.31
ATOM	809	CD2	TYR	99	-16.497	4.620	10.590	1.00	13.40
ATOM	810	CE2	TYR	99	-16.222	3.880	9.437	1.00	14.09
ATOM	811	CZ	TYR	99	-15.604	4.499	8.357	1.00	13.93
ATOM	812	OH	TYR	99	-15.250	3.750	7.254	1.00	16.39
ATOM	813	C	TYR	99	-18.090	7.309	13.732	1.00	11.30
ATOM	814	O	TYR	99	-18.224	8.507	13.984	1.00	11.78
ATOM	815	N	PRO	100	-18.076	6.377	14.706	1.00	10.91
ATOM	816	CD	PRO	100	-18.021	4.910	14.565	1.00	11.45
ATOM	817	CA	PRO	100	-18.253	6.745	16.115	1.00	10.77
ATOM	818	CB	PRO	100	-18.819	5.465	16.721	1.00	11.47
ATOM	819	CG	PRO	100	-18.046	4.433	16.020	1.00	11.97
ATOM	820	C	PRO	100	-16.997	7.205	16.847	1.00	9.85
ATOM	821	O	PRO	100	-17.074	7.694	17.975	1.00	10.01
ATOM	822	N	ALA	101	-15.853	7.040	16.192	1.00	9.97
ATOM	823	CA	ALA	101	-14.567	7.435	16.757	1.00	9.16
ATOM	824	CB	ALA	101	-14.197	6.529	17.942	1.00	9.95
ATOM	825	C	ALA	101	-13.537	7.300	15.653	1.00	8.68
ATOM	826	O	ALA	101	-13.837	6.791	14.564	1.00	9.27
ATOM	827	N	ALA	102	-12.317	7.756	15.924	1.00	7.79
ATOM	828	CA	ALA	102	-11.262	7.652	14.928	1.00	7.04
ATOM	829	CB	ALA	102	-11.464	8.711	13.863	1.00	7.86
ATOM	830	C	ALA	102	-9.884	7.802	15.541	1.00	7.06
ATOM	831	O	ALA	102	-9.726	8.466	16.561	1.00	6.93
ATOM	832	N	VAL	103	-8.893	7.150	14.941	1.00	6.76
ATOM	833	CA	VAL	103	-7.513	7.286	15.390	1.00	6.47
ATOM	834	CB	VAL	103	-6.753	5.950	15.410	1.00	6.79
ATOM	835	CG1	VAL	103	-5.305	6.203	15.819	1.00	7.90
ATOM	836	CG2	VAL	103	-7.398	4.967	16.389	1.00	7.20
ATOM	837	C	VAL	103	-6.862	8.189	14.345	1.00	7.38
ATOM	838	O	VAL	103	-6.790	7.828	13.169	1.00	7.79
ATOM	839	N	VAL	104	-6.390	9.351	14.790	1.00	7.31
ATOM	840	CA	VAL	104	-5.743	10.345	13.924	1.00	6.80
ATOM	841	CB	VAL	104	-5.999	11.758	14.474	1.00	6.60
ATOM	842	CG1	VAL	104	-5.409	12.800	13.535	1.00	9.75
ATOM	843	CG2	VAL	104	-7.517	11.964	14.658	1.00	8.12
ATOM	844	C	VAL	104	-4.234	10.082	13.841	1.00	7.14
ATOM	845	O	VAL	104	-3.544	10.028	14.856	1.00	6.83
ATOM	846	N	VAL	105	-3.729	9.933	12.619	1.00	6.94
ATOM	847	CA	VAL	105	-2.323	9.631	12.380	1.00	8.22
ATOM	848	CB	VAL	105	-2.177	8.175	11.846	1.00	8.31
ATOM	849	CG1	VAL	105	-.707	7.846	11.576	1.00	9.97
ATOM	850	CG2	VAL	105	-2.758	7.174	12.862	1.00	9.28
ATOM	851	C	VAL	105	-1.682	10.576	11.356	1.00	8.46
ATOM	852	O	VAL	105	-2.053	10.569	10.187	1.00	9.24
ATOM	853	N	GLU	106	-.715	11.382	11.789	1.00	8.82

ATOM	854	CA	GLU	106	-.006	12.284	10.872	1.00	10.03
ATOM	855	CB	GLU	106	.923	13.197	11.676	1.00	12.62
ATOM	856	CG	GLU	106	.198	14.195	12.553	1.00	18.74
ATOM	857	CD	GLU	106	.103	15.575	11.924	1.00	22.89
ATOM	858	OE1	GLU	106	.084	15.665	10.673	1.00	25.38
ATOM	859	OE2	GLU	106	.038	16.580	12.677	1.00	25.61
ATOM	860	C	GLU	106	.821	11.402	9.918	1.00	10.06
ATOM	861	O	GLU	106	1.300	10.329	10.321	1.00	9.56
ATOM	862	N	ASP	107	.991	11.866	8.675	1.00	10.64
ATOM	863	CA	ASP	107	1.728	11.135	7.636	1.00	11.81
ATOM	864	CB	ASP	107	1.582	11.860	6.288	1.00	14.69
ATOM	865	CG	ASP	107	2.350	13.182	6.236	1.00	17.04
ATOM	866	OD1	ASP	107	2.555	13.819	7.287	1.00	20.00
ATOM	867	OD2	ASP	107	2.745	13.611	5.128	1.00	21.03
ATOM	868	C	ASP	107	3.211	10.820	7.863	1.00	11.89
ATOM	869	O	ASP	107	3.816	10.123	7.054	1.00	11.94
ATOM	870	N	ASP	108	3.812	11.340	8.930	1.00	11.84
ATOM	871	CA	ASP	108	5.217	11.049	9.202	1.00	11.53
ATOM	872	CB	ASP	108	6.033	12.345	9.348	1.00	13.92
ATOM	873	CG	ASP	108	5.575	13.198	10.502	1.00	15.87
ATOM	874	OD1	ASP	108	4.441	12.977	10.998	1.00	16.09
ATOM	875	OD2	ASP	108	6.342	14.118	10.905	1.00	19.22
ATOM	876	C	ASP	108	5.387	10.159	10.438	1.00	10.17
ATOM	877	O	ASP	108	6.436	10.152	11.074	1.00	9.96
ATOM	878	N	LEU	109	4.344	9.399	10.754	1.00	8.52
ATOM	879	CA	LEU	109	4.382	8.471	11.881	1.00	8.40
ATOM	880	CB	LEU	109	3.148	8.629	12.770	1.00	9.34
ATOM	881	CG	LEU	109	2.957	9.979	13.472	1.00	9.58
ATOM	882	CD1	LEU	109	1.671	9.965	14.310	1.00	9.82
ATOM	883	CD2	LEU	109	4.178	10.275	14.335	1.00	11.12
ATOM	884	C	LEU	109	4.430	7.019	11.412	1.00	7.88
ATOM	885	O	LEU	109	3.683	6.619	10.515	1.00	8.33
ATOM	886	N	GLU	110	5.328	6.234	12.003	1.00	7.06
ATOM	887	CA	GLU	110	5.415	4.815	11.691	1.00	8.09
ATOM	888	CB	GLU	110	6.860	4.361	11.517	1.00	9.97
ATOM	889	CG	GLU	110	6.949	2.848	11.426	1.00	12.34
ATOM	890	CD	GLU	110	8.319	2.348	11.049	1.00	15.79
ATOM	891	OE1	GLU	110	8.975	3.007	10.221	1.00	16.61
ATOM	892	OE2	GLU	110	8.731	1.280	11.557	1.00	16.53
ATOM	893	C	GLU	110	4.812	4.105	12.899	1.00	7.72
ATOM	894	O	GLU	110	5.160	4.416	14.036	1.00	7.64
ATOM	895	N	VAL	111	3.900	3.172	12.662	1.00	6.91
ATOM	896	CA	VAL	111	3.250	2.482	13.779	1.00	7.11
ATOM	897	CB	VAL	111	1.770	2.170	13.465	1.00	6.84
ATOM	898	CG1	VAL	111	1.021	3.458	13.124	1.00	6.72
ATOM	899	CG2	VAL	111	1.687	1.169	12.334	1.00	7.62
ATOM	900	C	VAL	111	3.911	1.188	14.221	1.00	7.23
ATOM	901	O	VAL	111	4.567	.508	13.430	1.00	8.32
ATOM	902	N	ALA	112	3.709	.849	15.497	1.00	7.26
ATOM	903	CA	ALA	112	4.258	-.365	16.090	1.00	7.91
ATOM	904	CB	ALA	112	4.304	-.218	17.613	1.00	7.09
ATOM	905	C	ALA	112	3.396	-1.573	15.709	1.00	7.92
ATOM	906	O	ALA	112	2.249	-1.415	15.277	1.00	7.60
ATOM	907	N	PRO	113	3.929	-2.792	15.867	1.00	6.93
ATOM	908	CD	PRO	113	5.314	-3.140	16.232	1.00	8.97
ATOM	909	CA	PRO	113	3.165	-3.995	15.525	1.00	7.61
ATOM	910	CB	PRO	113	4.145	-5.130	15.823	1.00	8.86
ATOM	911	CG	PRO	113	5.481	-4.487	15.566	1.00	11.96
ATOM	912	C	PRO	113	1.860	-4.152	16.293	1.00	7.54
ATOM	913	O	PRO	113	.924	-4.750	15.770	1.00	8.06

ATOM	914	N	ASP	114	1.796	-3.644	17.529	1.00	7.44
ATOM	915	CA	ASP	114	.556	-3.755	18.302	1.00	6.79
ATOM	916	CB	ASP	114	.818	-4.265	19.730	1.00	7.74
ATOM	917	CG	ASP	114	1.946	-3.517	20.447	1.00	8.10
ATOM	918	OD1	ASP	114	2.450	-2.492	19.937	1.00	8.42
ATOM	919	OD2	ASP	114	2.328	-3.969	21.549	1.00	8.74
ATOM	920	C	ASP	114	-.253	-2.465	18.362	1.00	7.15
ATOM	921	O	ASP	114	-1.078	-2.279	19.250	1.00	6.63
ATOM	922	N	PHE	115	-.017	-1.587	17.398	1.00	5.88
ATOM	923	CA	PHE	115	-.739	-.312	17.303	1.00	6.49
ATOM	924	CB	PHE	115	-.283	.408	16.027	1.00	7.06
ATOM	925	CG	PHE	115	-1.044	1.682	15.717	1.00	7.08
ATOM	926	CD1	PHE	115	-.632	2.906	16.238	1.00	7.32
ATOM	927	CD2	PHE	115	-2.148	1.659	14.861	1.00	8.19
ATOM	928	CE1	PHE	115	-1.305	4.098	15.903	1.00	7.12
ATOM	929	CE2	PHE	115	-2.831	2.853	14.523	1.00	7.40
ATOM	930	CZ	PHE	115	-2.400	4.069	15.048	1.00	7.26
ATOM	931	C	PHE	115	-2.262	-.524	17.275	1.00	6.27
ATOM	932	O	PHE	115	-3.005	.143	18.014	1.00	5.65
ATOM	933	N	PHE	116	-2.723	-1.447	16.429	1.00	6.43
ATOM	934	CA	PHE	116	-4.158	-1.707	16.310	1.00	6.62
ATOM	935	CB	PHE	116	-4.450	-2.499	15.027	1.00	7.53
ATOM	936	CG	PHE	116	-4.047	-1.774	13.770	1.00	7.90
ATOM	937	CD1	PHE	116	-2.788	-1.979	13.205	1.00	7.81
ATOM	938	CD2	PHE	116	-4.921	-.886	13.161	1.00	7.23
ATOM	939	CE1	PHE	116	-2.411	-1.307	12.041	1.00	8.33
ATOM	940	CE2	PHE	116	-4.558	-.207	11.999	1.00	8.55
ATOM	941	CZ	PHE	116	-3.294	-.423	11.437	1.00	7.71
ATOM	942	C	PHE	116	-4.711	-2.423	17.531	1.00	6.03
ATOM	943	O	PHE	116	-5.787	-2.084	18.012	1.00	6.90
ATOM	944	N	GLU	117	-3.961	-3.396	18.035	1.00	6.55
ATOM	945	CA	GLU	117	-4.359	-4.148	19.213	1.00	6.50
ATOM	946	CB	GLU	117	-3.267	-5.180	19.535	1.00	7.64
ATOM	947	CG	GLU	117	-3.469	-6.013	20.816	1.00	8.61
ATOM	948	CD	GLU	117	-4.479	-7.133	20.680	1.00	8.79
ATOM	949	OE1	GLU	117	-4.892	-7.439	19.543	1.00	9.51
ATOM	950	OE2	GLU	117	-4.854	-7.728	21.719	1.00	8.74
ATOM	951	C	GLU	117	-4.552	-3.172	20.370	1.00	6.50
ATOM	952	O	GLU	117	-5.502	-3.280	21.144	1.00	6.96
ATOM	953	N	TYR	118	-3.636	-2.213	20.479	1.00	6.11
ATOM	954	CA	TYR	118	-3.670	-1.195	21.540	1.00	5.31
ATOM	955	CB	TYR	118	-2.445	-.283	21.392	1.00	5.34
ATOM	956	CG	TYR	118	-2.398	.922	22.313	1.00	5.58
ATOM	957	CD1	TYR	118	-2.307	.773	23.694	1.00	5.81
ATOM	958	CE1	TYR	118	-2.208	1.876	24.536	1.00	6.06
ATOM	959	CD2	TYR	118	-2.394	2.214	21.790	1.00	5.76
ATOM	960	CE2	TYR	118	-2.297	3.336	22.624	1.00	5.76
ATOM	961	CZ	TYR	118	-2.200	3.157	24.000	1.00	5.05
ATOM	962	OH	TYR	118	-2.078	4.254	24.836	1.00	6.90
ATOM	963	C	TYR	118	-4.958	-.368	21.512	1.00	5.32
ATOM	964	O	TYR	118	-5.645	-.219	22.531	1.00	6.21
ATOM	965	N	PHE	119	-5.307	.154	20.348	1.00	5.61
ATOM	966	CA	PHE	119	-6.522	.942	20.277	1.00	5.83
ATOM	967	CB	PHE	119	-6.523	1.788	19.007	1.00	6.69
ATOM	968	CG	PHE	119	-5.595	2.949	19.093	1.00	6.79
ATOM	969	CD1	PHE	119	-4.399	2.965	18.390	1.00	7.03
ATOM	970	CD2	PHE	119	-5.888	4.016	19.950	1.00	6.34
ATOM	971	CE1	PHE	119	-3.497	4.035	18.543	1.00	7.10
ATOM	972	CE2	PHE	119	-5.005	5.076	20.104	1.00	7.50
ATOM	973	CZ	PHE	119	-3.806	5.088	19.401	1.00	7.69

ATOM	974	C	PHE	119	-7.783	.108	20.423	1.00	6.63
ATOM	975	O	PHE	119	-8.771	.573	20.995	1.00	8.58
ATOM	976	N	GLN	120	-7.756	-1.132	19.954	1.00	6.90
ATOM	977	CA	GLN	120	-8.935	-1.980	20.096	1.00	8.05
ATOM	978	CB	GLN	120	-8.713	-3.323	19.383	1.00	10.25
ATOM	979	CG	GLN	120	-9.954	-4.218	19.251	1.00	13.92
ATOM	980	CD	GLN	120	-11.052	-3.601	18.384	1.00	15.62
ATOM	981	OE1	GLN	120	-12.188	-3.441	18.823	1.00	19.48
ATOM	982	NE2	GLN	120	-10.712	-3.265	17.147	1.00	18.32
ATOM	983	C	GLN	120	-9.209	-2.211	21.585	1.00	7.92
ATOM	984	O	GLN	120	-10.355	-2.183	22.038	1.00	8.72
ATOM	985	N	ALA	121	-8.145	-2.409	22.347	1.00	7.70
ATOM	986	CA	ALA	121	-8.256	-2.682	23.777	1.00	8.08
ATOM	987	CB	ALA	121	-6.940	-3.249	24.281	1.00	8.52
ATOM	988	C	ALA	121	-8.640	-1.484	24.633	1.00	8.17
ATOM	989	O	ALA	121	-9.349	-1.622	25.619	1.00	8.48
ATOM	990	N	THR	122	-8.153	-.307	24.267	1.00	7.78
ATOM	991	CA	THR	122	-8.423	.888	25.046	1.00	7.97
ATOM	992	CB	THR	122	-7.201	1.818	24.989	1.00	7.90
ATOM	993	OG1	THR	122	-6.838	2.031	23.621	1.00	7.16
ATOM	994	CG2	THR	122	-6.008	1.174	25.699	1.00	8.16
ATOM	995	C	THR	122	-9.672	1.673	24.669	1.00	8.48
ATOM	996	O	THR	122	-10.125	2.523	25.440	1.00	8.57
ATOM	997	N	TYR	123	-10.228	1.405	23.491	1.00	8.46
ATOM	998	CA	TYR	123	-11.439	2.099	23.059	1.00	8.68
ATOM	999	CB	TYR	123	-11.828	1.595	21.662	1.00	9.87
ATOM	1000	CG	TYR	123	-13.111	2.144	21.068	1.00	11.57
ATOM	1001	CD1	TYR	123	-13.468	3.483	21.207	1.00	11.70
ATOM	1002	CE1	TYR	123	-14.623	3.983	20.599	1.00	12.19
ATOM	1003	CD2	TYR	123	-13.940	1.319	20.308	1.00	13.45
ATOM	1004	CE2	TYR	123	-15.092	1.811	19.689	1.00	13.82
ATOM	1005	CZ	TYR	123	-15.420	3.149	19.843	1.00	12.95
ATOM	1006	OH	TYR	123	-16.541	3.654	19.202	1.00	15.32
ATOM	1007	C	TYR	123	-12.577	1.920	24.083	1.00	9.48
ATOM	1008	O	TYR	123	-13.267	2.878	24.427	1.00	8.67
ATOM	1009	N	PRO	124	-12.786	.691	24.591	1.00	9.37
ATOM	1010	CD	PRO	124	-12.213	-.604	24.175	1.00	10.62
ATOM	1011	CA	PRO	124	-13.871	.521	25.573	1.00	10.34
ATOM	1012	CB	PRO	124	-13.872	-.995	25.859	1.00	11.01
ATOM	1013	CG	PRO	124	-12.547	-1.492	25.339	1.00	12.63
ATOM	1014	C	PRO	124	-13.653	1.381	26.826	1.00	10.14
ATOM	1015	O	PRO	124	-14.621	1.877	27.424	1.00	10.56
ATOM	1016	N	LEU	125	-12.392	1.562	27.226	1.00	9.88
ATOM	1017	CA	LEU	125	-12.081	2.409	28.381	1.00	10.66
ATOM	1018	CB	LEU	125	-10.572	2.384	28.720	1.00	13.15
ATOM	1019	CG	LEU	125	-10.024	1.238	29.577	1.00	16.82
ATOM	1020	CD1	LEU	125	-10.343	1.472	31.048	1.00	17.41
ATOM	1021	CD2	LEU	125	-10.606	-.067	29.110	1.00	17.36
ATOM	1022	C	LEU	125	-12.489	3.856	28.085	1.00	9.99
ATOM	1023	O	LEU	125	-13.075	4.526	28.922	1.00	10.44
ATOM	1024	N	LEU	126	-12.165	4.335	26.891	1.00	9.83
ATOM	1025	CA	LEU	126	-12.500	5.698	26.503	1.00	9.02
ATOM	1026	CB	LEU	126	-11.882	6.005	25.134	1.00	8.02
ATOM	1027	CG	LEU	126	-12.087	7.413	24.578	1.00	7.49
ATOM	1028	CD1	LEU	126	-11.549	8.473	25.559	1.00	8.32
ATOM	1029	CD2	LEU	126	-11.378	7.502	23.231	1.00	8.74
ATOM	1030	C	LEU	126	-14.010	5.892	26.466	1.00	9.68
ATOM	1031	O	LEU	126	-14.523	6.920	26.880	1.00	9.94
ATOM	1032	N	LYS	127	-14.727	4.905	25.951	1.00	10.67
ATOM	1033	CA	LYS	127	-16.181	5.001	25.910	1.00	12.13

ATOM	1034	CB	LYS	127	-16.764	3.831	25.112	1.00	13.06
ATOM	1035	CG	LYS	127	-16.605	3.971	23.623	1.00	14.44
ATOM	1036	CD	LYS	127	-17.279	2.850	22.846	1.00	17.49
ATOM	1037	CE	LYS	127	-16.484	1.562	22.924	1.00	18.56
ATOM	1038	NZ	LYS	127	-17.039	.506	22.023	1.00	20.98
ATOM	1039	C	LYS	127	-16.802	5.003	27.307	1.00	12.68
ATOM	1040	O	LYS	127	-17.782	5.716	27.548	1.00	13.23
ATOM	1041	N	ALA	128	-16.219	4.246	28.236	1.00	13.11
ATOM	1042	CA	ALA	128	-16.786	4.126	29.575	1.00	14.17
ATOM	1043	CB	ALA	128	-16.545	2.706	30.100	1.00	16.00
ATOM	1044	C	ALA	128	-16.365	5.148	30.624	1.00	15.14
ATOM	1045	O	ALA	128	-17.113	5.392	31.581	1.00	16.96
ATOM	1046	N	ASP	129	-15.206	5.774	30.449	1.00	13.30
ATOM	1047	CA	ASP	129	-14.713	6.726	31.448	1.00	12.36
ATOM	1048	CB	ASP	129	-13.270	6.366	31.825	1.00	12.73
ATOM	1049	CG	ASP	129	-12.774	7.142	33.021	1.00	13.33
ATOM	1050	OD1	ASP	129	-13.469	8.101	33.418	1.00	13.06
ATOM	1051	OD2	ASP	129	-11.682	6.814	33.562	1.00	15.51
ATOM	1052	C	ASP	129	-14.765	8.173	30.956	1.00	11.84
ATOM	1053	O	ASP	129	-13.919	8.596	30.164	1.00	10.96
ATOM	1054	N	PRO	130	-15.736	8.965	31.443	1.00	11.10
ATOM	1055	CD	PRO	130	-16.816	8.574	32.370	1.00	11.15
ATOM	1056	CA	PRO	130	-15.879	10.362	31.030	1.00	10.61
ATOM	1057	CB	PRO	130	-17.231	10.757	31.632	1.00	11.99
ATOM	1058	CG	PRO	130	-17.293	9.898	32.878	1.00	12.73
ATOM	1059	C	PRO	130	-14.739	11.292	31.439	1.00	10.03
ATOM	1060	O	PRO	130	-14.643	12.435	30.948	1.00	10.59
ATOM	1061	N	SER	131	-13.872	10.811	32.324	1.00	8.99
ATOM	1062	CA	SER	131	-12.723	11.606	32.755	1.00	9.12
ATOM	1063	CB	SER	131	-12.262	11.201	34.166	1.00	9.91
ATOM	1064	OG	SER	131	-11.707	9.899	34.195	1.00	10.84
ATOM	1065	C	SER	131	-11.581	11.461	31.740	1.00	8.46
ATOM	1066	O	SER	131	-10.552	12.136	31.847	1.00	8.86
ATOM	1067	N	LEU	132	-11.760	10.564	30.770	1.00	7.79
ATOM	1068	CA	LEU	132	-10.778	10.394	29.691	1.00	7.36
ATOM	1069	CB	LEU	132	-10.590	8.916	29.344	1.00	8.15
ATOM	1070	CG	LEU	132	-9.892	8.028	30.348	1.00	7.90
ATOM	1071	CD1	LEU	132	-9.872	6.587	29.778	1.00	8.80
ATOM	1072	CD2	LEU	132	-8.464	8.532	30.601	1.00	9.13
ATOM	1073	C	LEU	132	-11.319	11.078	28.440	1.00	8.29
ATOM	1074	O	LEU	132	-12.528	11.029	28.182	1.00	8.71
ATOM	1075	N	TRP	133	-10.449	11.720	27.661	1.00	6.83
ATOM	1076	CA	TRP	133	-10.913	12.307	26.418	1.00	6.67
ATOM	1077	CB	TRP	133	-10.989	13.849	26.519	1.00	6.62
ATOM	1078	CG	TRP	133	-9.717	14.635	26.389	1.00	7.14
ATOM	1079	CD2	TRP	133	-9.598	15.977	25.889	1.00	7.20
ATOM	1080	CE2	TRP	133	-8.242	16.344	26.004	1.00	6.33
ATOM	1081	CE3	TRP	133	-10.510	16.902	25.358	1.00	7.85
ATOM	1082	CD1	TRP	133	-8.466	14.256	26.774	1.00	7.23
ATOM	1083	NE1	TRP	133	-7.577	15.275	26.547	1.00	6.53
ATOM	1084	CZ2	TRP	133	-7.769	17.600	25.604	1.00	7.96
ATOM	1085	CZ3	TRP	133	-10.042	18.154	24.959	1.00	8.61
ATOM	1086	CH2	TRP	133	-8.681	18.486	25.084	1.00	7.98
ATOM	1087	C	TRP	133	-10.107	11.809	25.217	1.00	6.93
ATOM	1088	O	TRP	133	-10.409	12.135	24.073	1.00	6.69
ATOM	1089	N	CYS	134	-9.101	10.981	25.480	1.00	6.96
ATOM	1090	CA	CYS	134	-8.312	10.395	24.393	1.00	6.36
ATOM	1091	C	CYS	134	-7.422	9.247	24.807	1.00	6.40
ATOM	1092	O	CYS	134	-7.199	8.995	25.990	1.00	5.47
ATOM	1093	CB	CYS	134	-7.443	11.474	23.729	1.00	8.82

ATOM	1094	SG	CYS	134	-5.616	11.492	23.979	1.00	11.44
ATOM	1095	N	VAL	135	-6.948	8.521	23.803	1.00	6.39
ATOM	1096	CA	VAL	135	-5.980	7.460	24.016	1.00	6.39
ATOM	1097	CB	VAL	135	-6.515	6.068	23.672	1.00	5.84
ATOM	1098	CG1	VAL	135	-5.379	5.058	23.756	1.00	7.18
ATOM	1099	CG2	VAL	135	-7.625	5.663	24.649	1.00	7.00
ATOM	1100	C	VAL	135	-4.895	7.838	23.011	1.00	6.94
ATOM	1101	O	VAL	135	-5.192	8.066	21.833	1.00	6.85
ATOM	1102	N	SER	136	-3.648	7.932	23.477	1.00	5.34
ATOM	1103	CA	SER	136	-2.534	8.285	22.604	1.00	5.91
ATOM	1104	CB	SER	136	-1.874	9.585	23.074	1.00	5.91
ATOM	1105	OG	SER	136	-.721	9.866	22.284	1.00	6.37
ATOM	1106	C	SER	136	-1.502	7.174	22.588	1.00	5.57
ATOM	1107	O	SER	136	-1.316	6.482	23.586	1.00	5.36
ATOM	1108	N	ALA	137	-.843	7.009	21.447	1.00	5.87
ATOM	1109	CA	ALA	137	.203	6.009	21.290	1.00	5.91
ATOM	1110	CB	ALA	137	.308	5.596	19.806	1.00	6.92
ATOM	1111	C	ALA	137	1.548	6.580	21.743	1.00	6.32
ATOM	1112	O	ALA	137	2.530	5.858	21.810	1.00	6.83
ATOM	1113	N	TRP	138	1.585	7.861	22.095	1.00	5.76
ATOM	1114	CA	TRP	138	2.857	8.531	22.417	1.00	6.20
ATOM	1115	CB	TRP	138	2.861	9.891	21.683	1.00	7.40
ATOM	1116	CG	TRP	138	4.191	10.622	21.603	1.00	8.17
ATOM	1117	CD2	TRP	138	5.178	10.494	20.570	1.00	8.96
ATOM	1118	CE2	TRP	138	6.218	11.409	20.863	1.00	9.96
ATOM	1119	CE3	TRP	138	5.282	9.697	19.421	1.00	8.97
ATOM	1120	CD1	TRP	138	4.664	11.579	22.466	1.00	10.04
ATOM	1121	NE1	TRP	138	5.884	12.062	22.020	1.00	9.12
ATOM	1122	CZ2	TRP	138	7.352	11.548	20.043	1.00	10.71
ATOM	1123	CZ3	TRP	138	6.417	9.837	18.601	1.00	10.53
ATOM	1124	CH2	TRP	138	7.433	10.760	18.924	1.00	10.63
ATOM	1125	C	TRP	138	3.291	8.763	23.860	1.00	7.18
ATOM	1126	O	TRP	138	2.525	9.267	24.680	1.00	7.82
ATOM	1127	N	ASN	139	4.539	8.393	24.155	1.00	7.29
ATOM	1128	CA	ASN	139	5.148	8.670	25.459	1.00	7.67
ATOM	1129	CB	ASN	139	5.929	7.453	25.975	1.00	7.59
ATOM	1130	CG	ASN	139	6.663	7.731	27.289	1.00	7.82
ATOM	1131	OD1	ASN	139	6.685	8.850	27.781	1.00	7.63
ATOM	1132	ND2	ASN	139	7.274	6.702	27.852	1.00	6.80
ATOM	1133	C	ASN	139	6.124	9.845	25.223	1.00	8.08
ATOM	1134	O	ASN	139	7.191	9.670	24.626	1.00	7.12
ATOM	1135	N	ASP	140	5.769	11.038	25.690	1.00	8.24
ATOM	1136	CA	ASP	140	6.635	12.198	25.500	1.00	9.35
ATOM	1137	CB	ASP	140	5.951	13.444	26.065	1.00	11.81
ATOM	1138	CG	ASP	140	4.834	13.967	25.154	1.00	14.17
ATOM	1139	OD1	ASP	140	5.139	14.622	24.133	1.00	16.16
ATOM	1140	OD2	ASP	140	3.645	13.720	25.447	1.00	16.99
ATOM	1141	C	ASP	140	8.081	12.027	26.045	1.00	9.97
ATOM	1142	O	ASP	140	9.021	12.666	25.553	1.00	10.29
ATOM	1143	N	ASN	141	8.278	11.155	27.030	1.00	9.29
ATOM	1144	CA	ASN	141	9.626	10.894	27.528	1.00	9.92
ATOM	1145	CB	ASN	141	9.708	11.071	29.042	1.00	10.62
ATOM	1146	CG	ASN	141	9.579	12.506	29.458	1.00	11.57
ATOM	1147	OD1	ASN	141	10.393	13.353	29.074	1.00	12.39
ATOM	1148	ND2	ASN	141	8.562	12.798	30.249	1.00	11.15
ATOM	1149	C	ASN	141	9.949	9.453	27.175	1.00	10.26
ATOM	1150	O	ASN	141	10.454	8.703	27.996	1.00	11.41
ATOM	1151	N	GLY	142	9.689	9.075	25.926	1.00	8.78
ATOM	1152	CA	GLY	142	9.902	7.696	25.533	1.00	8.32
ATOM	1153	C	GLY	142	11.208	7.297	24.875	1.00	8.26

ATOM	1154	O	GLY	142	11.217	6.373	24.063	1.00	8.28
ATOM	1155	N	LYS	143	12.305	7.970	25.186	1.00	8.56
ATOM	1156	CA	LYS	143	13.566	7.549	24.584	1.00	10.27
ATOM	1157	CB	LYS	143	14.673	8.561	24.812	1.00	12.79
ATOM	1158	CG	LYS	143	14.880	8.938	26.245	1.00	16.83
ATOM	1159	CD	LYS	143	16.055	9.912	26.358	1.00	20.40
ATOM	1160	CE	LYS	143	15.912	11.086	25.384	1.00	20.81
ATOM	1161	NZ	LYS	143	17.094	12.020	25.423	1.00	22.77
ATOM	1162	C	LYS	143	13.941	6.225	25.228	1.00	9.41
ATOM	1163	O	LYS	143	13.541	5.924	26.351	1.00	9.21
ATOM	1164	N	GLU	144	14.726	5.443	24.512	1.00	10.01
ATOM	1165	CA	GLU	144	15.116	4.130	24.971	1.00	11.30
ATOM	1166	CB	GLU	144	16.148	3.568	24.012	1.00	15.41
ATOM	1167	CG	GLU	144	16.456	2.121	24.204	1.00	20.56
ATOM	1168	CD	GLU	144	17.510	1.675	23.213	1.00	24.26
ATOM	1169	OE1	GLU	144	17.176	1.538	22.007	1.00	26.09
ATOM	1170	OE2	GLU	144	18.681	1.485	23.640	1.00	27.96
ATOM	1171	C	GLU	144	15.633	4.013	26.402	1.00	11.49
ATOM	1172	O	GLU	144	15.262	3.084	27.115	1.00	10.97
ATOM	1173	N	GLN	145	16.481	4.937	26.830	1.00	10.88
ATOM	1174	CA	GLN	145	17.021	4.833	28.172	1.00	11.67
ATOM	1175	CB	GLN	145	18.313	5.640	28.274	1.00	13.90
ATOM	1176	CG	GLN	145	19.459	5.071	27.427	1.00	17.26
ATOM	1177	CD	GLN	145	19.815	3.623	27.787	1.00	19.75
ATOM	1178	OE1	GLN	145	19.991	3.266	28.973	1.00	21.30
ATOM	1179	NE2	GLN	145	19.930	2.782	26.772	1.00	21.25
ATOM	1180	C	GLN	145	16.058	5.268	29.255	1.00	11.28
ATOM	1181	O	GLN	145	16.372	5.184	30.448	1.00	11.87
ATOM	1182	N	MET	146	14.875	5.721	28.857	1.00	9.49
ATOM	1183	CA	MET	146	13.925	6.183	29.846	1.00	10.71
ATOM	1184	CB	MET	146	13.598	7.648	29.585	1.00	13.91
ATOM	1185	CG	MET	146	14.814	8.547	29.824	1.00	18.48
ATOM	1186	SD	MET	146	14.531	10.209	29.312	1.00	25.79
ATOM	1187	CE	MET	146	13.495	10.753	30.558	1.00	22.78
ATOM	1188	C	MET	146	12.661	5.370	29.954	1.00	9.53
ATOM	1189	O	MET	146	11.732	5.767	30.651	1.00	9.31
ATOM	1190	N	VAL	147	12.639	4.236	29.262	1.00	8.91
ATOM	1191	CA	VAL	147	11.495	3.335	29.298	1.00	8.59
ATOM	1192	CB	VAL	147	10.769	3.238	27.924	1.00	8.51
ATOM	1193	CG1	VAL	147	10.350	4.608	27.472	1.00	9.27
ATOM	1194	CG2	VAL	147	11.665	2.554	26.891	1.00	9.93
ATOM	1195	C	VAL	147	11.955	1.935	29.701	1.00	9.07
ATOM	1196	O	VAL	147	13.104	1.537	29.434	1.00	9.65
ATOM	1197	N	ASP	148	11.056	1.206	30.350	1.00	8.43
ATOM	1198	CA	ASP	148	11.327	-.147	30.809	1.00	8.38
ATOM	1199	CB	ASP	148	10.534	-.460	32.083	1.00	9.83
ATOM	1200	CG	ASP	148	10.947	-1.783	32.720	1.00	11.52
ATOM	1201	OD1	ASP	148	11.645	-2.592	32.054	1.00	11.93
ATOM	1202	OD2	ASP	148	10.567	-2.027	33.896	1.00	14.00
ATOM	1203	C	ASP	148	10.921	-1.124	29.727	1.00	8.99
ATOM	1204	O	ASP	148	9.728	-1.424	29.552	1.00	9.02
ATOM	1205	N	SER	149	11.921	-1.657	29.033	1.00	9.31
ATOM	1206	CA	SER	149	11.664	-2.587	27.949	1.00	10.55
ATOM	1207	CB	SER	149	12.939	-2.810	27.139	1.00	12.64
ATOM	1208	OG	SER	149	13.915	-3.437	27.949	1.00	18.01
ATOM	1209	C	SER	149	11.111	-3.916	28.428	1.00	9.89
ATOM	1210	O	SER	149	10.686	-4.729	27.611	1.00	10.17
ATOM	1211	N	SER	150	11.127	-4.161	29.740	1.00	9.75
ATOM	1212	CA	SER	150	10.570	-5.406	30.264	1.00	9.43
ATOM	1213	CB	SER	150	11.288	-5.856	31.550	1.00	10.84

ATOM	1214	OG	SER	150	10.990	-5.002	32.639	1.00	12.22
ATOM	1215	C	SER	150	9.084	-5.221	30.568	1.00	9.62
ATOM	1216	O	SER	150	8.409	-6.162	30.960	1.00	9.90
ATOM	1217	N	LYS	151	8.578	-4.006	30.387	1.00	7.76
ATOM	1218	CA	LYS	151	7.165	-3.737	30.656	1.00	7.60
ATOM	1219	CB	LYS	151	7.027	-2.861	31.910	1.00	8.05
ATOM	1220	CG	LYS	151	7.289	-3.589	33.243	1.00	7.72
ATOM	1221	CD	LYS	151	6.250	-4.682	33.577	1.00	8.36
ATOM	1222	CE	LYS	151	4.854	-4.128	33.862	1.00	9.62
ATOM	1223	NZ	LYS	151	3.939	-5.244	34.274	1.00	7.59
ATOM	1224	C	LYS	151	6.468	-3.072	29.464	1.00	7.65
ATOM	1225	O	LYS	151	5.850	-2.006	29.590	1.00	7.71
ATOM	1226	N	PRO	152	6.553	-3.700	28.277	1.00	7.60
ATOM	1227	CD	PRO	152	7.176	-4.995	27.949	1.00	7.43
ATOM	1228	CA	PRO	152	5.902	-3.111	27.107	1.00	7.61
ATOM	1229	CB	PRO	152	6.329	-4.037	25.968	1.00	7.92
ATOM	1230	CG	PRO	152	6.462	-5.375	26.664	1.00	8.72
ATOM	1231	C	PRO	152	4.383	-3.026	27.242	1.00	7.09
ATOM	1232	O	PRO	152	3.737	-2.312	26.482	1.00	7.12
ATOM	1233	N	GLU	153	3.816	-3.739	28.214	1.00	6.68
ATOM	1234	CA	GLU	153	2.361	-3.727	28.402	1.00	7.04
ATOM	1235	CB	GLU	153	1.886	-5.083	28.971	1.00	8.54
ATOM	1236	CG	GLU	153	2.223	-5.293	30.446	1.00	8.84
ATOM	1237	CD	GLU	153	3.610	-5.911	30.686	1.00	10.66
ATOM	1238	OE1	GLU	153	4.561	-5.641	29.916	1.00	10.13
ATOM	1239	OE2	GLU	153	3.751	-6.681	31.664	1.00	11.15
ATOM	1240	C	GLU	153	1.872	-2.601	29.336	1.00	7.41
ATOM	1241	O	GLU	153	.694	-2.304	29.388	1.00	6.96
ATOM	1242	N	LEU	154	2.786	-1.976	30.065	1.00	7.43
ATOM	1243	CA	LEU	154	2.408	-.945	31.024	1.00	6.92
ATOM	1244	CB	LEU	154	3.615	-.638	31.908	1.00	6.25
ATOM	1245	CG	LEU	154	3.323	.330	33.058	1.00	7.81
ATOM	1246	CD1	LEU	154	2.170	-.204	33.909	1.00	9.33
ATOM	1247	CD2	LEU	154	4.585	.491	33.903	1.00	9.13
ATOM	1248	C	LEU	154	1.832	.359	30.438	1.00	6.47
ATOM	1249	O	LEU	154	2.426	.964	29.549	1.00	6.52
ATOM	1250	N	LEU	155	.670	.776	30.949	1.00	6.07
ATOM	1251	CA	LEU	155	.014	2.002	30.487	1.00	5.42
ATOM	1252	CB	LEU	155	-1.352	1.684	29.865	1.00	5.69
ATOM	1253	CG	LEU	155	-1.341	.653	28.736	1.00	4.65
ATOM	1254	CD1	LEU	155	-2.785	.471	28.242	1.00	6.95
ATOM	1255	CD2	LEU	155	-.430	1.109	27.595	1.00	7.05
ATOM	1256	C	LEU	155	-.185	2.989	31.639	1.00	5.52
ATOM	1257	O	LEU	155	-.132	2.612	32.802	1.00	6.33
ATOM	1258	N	TYR	156	-.448	4.245	31.292	1.00	5.08
ATOM	1259	CA	TYR	156	-.624	5.321	32.273	1.00	5.60
ATOM	1260	CB	TYR	156	.641	6.187	32.348	1.00	6.03
ATOM	1261	CG	TYR	156	1.907	5.508	32.785	1.00	6.52
ATOM	1262	CD1	TYR	156	2.657	4.736	31.898	1.00	7.20
ATOM	1263	CE1	TYR	156	3.853	4.150	32.293	1.00	7.15
ATOM	1264	CD2	TYR	156	2.375	5.673	34.078	1.00	7.12
ATOM	1265	CE2	TYR	156	3.572	5.087	34.490	1.00	7.82
ATOM	1266	CZ	TYR	156	4.303	4.333	33.591	1.00	8.24
ATOM	1267	OH	TYR	156	5.499	3.787	33.983	1.00	8.82
ATOM	1268	C	TYR	156	-1.726	6.289	31.872	1.00	5.57
ATOM	1269	O	TYR	156	-2.215	6.251	30.747	1.00	6.98
ATOM	1270	N	ARG	157	-2.112	7.149	32.811	1.00	6.01
ATOM	1271	CA	ARG	157	-3.038	8.231	32.506	1.00	6.58
ATOM	1272	CB	ARG	157	-4.099	8.431	33.613	1.00	7.55
ATOM	1273	CG	ARG	157	-5.150	7.344	33.695	1.00	8.82

ATOM	1274	CD	ARG	157	-6.086	7.550	34.909	1.00	10.83
ATOM	1275	NE	ARG	157	-6.995	8.680	34.761	1.00	12.60
ATOM	1276	CZ	ARG	157	-8.252	8.612	34.310	1.00	11.74
ATOM	1277	NH1	ARG	157	-8.797	7.457	33.946	1.00	11.08
ATOM	1278	NH2	ARG	157	-8.965	9.718	34.224	1.00	12.96
ATOM	1279	C	ARG	157	-2.106	9.454	32.453	1.00	6.91
ATOM	1280	O	ARG	157	-1.074	9.500	33.145	1.00	7.31
ATOM	1281	N	THR	158	-2.447	10.434	31.619	1.00	6.75
ATOM	1282	CA	THR	158	-1.647	11.657	31.506	1.00	6.89
ATOM	1283	CB	THR	158	-.635	11.613	30.316	1.00	7.54
ATOM	1284	OG1	THR	158	.061	12.864	30.247	1.00	8.96
ATOM	1285	CG2	THR	158	-1.339	11.389	28.989	1.00	8.06
ATOM	1286	C	THR	158	-2.573	12.848	31.290	1.00	7.42
ATOM	1287	O	THR	158	-3.592	12.728	30.633	1.00	7.31
ATOM	1288	N	ASP	159	-2.229	13.989	31.875	1.00	6.73
ATOM	1289	CA	ASP	159	-3.034	15.199	31.720	1.00	7.70
ATOM	1290	CB	ASP	159	-2.889	16.111	32.945	1.00	6.88
ATOM	1291	CG	ASP	159	-3.635	15.590	34.141	1.00	8.75
ATOM	1292	OD1	ASP	159	-3.117	15.700	35.281	1.00	8.80
ATOM	1293	OD2	ASP	159	-4.754	15.078	33.944	1.00	10.09
ATOM	1294	C	ASP	159	-2.578	15.963	30.500	1.00	7.79
ATOM	1295	O	ASP	159	-3.252	16.905	30.058	1.00	9.31
ATOM	1296	N	PHE	160	-1.423	15.569	29.969	1.00	7.70
ATOM	1297	CA	PHE	160	-.842	16.222	28.794	1.00	7.99
ATOM	1298	CB	PHE	160	.692	16.209	28.914	1.00	8.75
ATOM	1299	CG	PHE	160	1.385	17.119	27.937	1.00	9.18
ATOM	1300	CD1	PHE	160	1.725	18.422	28.295	1.00	10.08
ATOM	1301	CD2	PHE	160	1.659	16.683	26.647	1.00	9.70
ATOM	1302	CE1	PHE	160	2.328	19.270	27.377	1.00	11.23
ATOM	1303	CE2	PHE	160	2.264	17.539	25.721	1.00	10.04
ATOM	1304	CZ	PHE	160	2.594	18.818	26.083	1.00	11.74
ATOM	1305	C	PHE	160	-1.260	15.518	27.490	1.00	8.42
ATOM	1306	O	PHE	160	-.781	14.418	27.201	1.00	9.13
ATOM	1307	N	PHE	161	-2.141	16.151	26.715	1.00	7.35
ATOM	1308	CA	PHE	161	-2.600	15.604	25.431	1.00	7.31
ATOM	1309	CB	PHE	161	-3.600	16.568	24.787	1.00	7.43
ATOM	1310	CG	PHE	161	-3.929	16.235	23.366	1.00	7.68
ATOM	1311	CD1	PHE	161	-4.549	15.026	23.039	1.00	7.44
ATOM	1312	CD2	PHE	161	-3.595	17.120	22.341	1.00	7.71
ATOM	1313	CE1	PHE	161	-4.828	14.703	21.701	1.00	8.96
ATOM	1314	CE2	PHE	161	-3.867	16.812	21.017	1.00	8.56
ATOM	1315	CZ	PHE	161	-4.485	15.601	20.685	1.00	8.87
ATOM	1316	C	PHE	161	-1.378	15.458	24.530	1.00	7.61
ATOM	1317	O	PHE	161	-.807	16.461	24.081	1.00	8.68
ATOM	1318	N	PRO	162	-.978	14.214	24.211	1.00	7.85
ATOM	1319	CD	PRO	162	-1.430	12.930	24.773	1.00	7.93
ATOM	1320	CA	PRO	162	.206	14.019	23.365	1.00	8.55
ATOM	1321	CB	PRO	162	.714	12.623	23.767	1.00	9.21
ATOM	1322	CG	PRO	162	-.120	12.205	24.956	1.00	9.29
ATOM	1323	C	PRO	162	.049	14.091	21.857	1.00	9.66
ATOM	1324	O	PRO	162	1.030	14.376	21.157	1.00	11.01
ATOM	1325	N	GLY	163	-1.160	13.829	21.359	1.00	9.98
ATOM	1326	CA	GLY	163	-1.403	13.787	19.919	1.00	9.33
ATOM	1327	C	GLY	163	-.578	12.613	19.392	1.00	8.97
ATOM	1328	O	GLY	163	-.511	11.566	20.045	1.00	9.22
ATOM	1329	N	LEU	164	.031	12.770	18.221	1.00	7.98
ATOM	1330	CA	LEU	164	.917	11.753	17.639	1.00	7.75
ATOM	1331	CB	LEU	164	2.285	11.829	18.338	1.00	9.13
ATOM	1332	CG	LEU	164	2.970	13.189	18.143	1.00	9.81
ATOM	1333	CD1	LEU	164	4.164	13.331	19.063	1.00	10.84

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ATOM   1334  CD2 LEU   164       3.380  13.325  16.690  1.00 11.12
ATOM   1335  C   LEU   164        .382  10.317  17.679  1.00  7.60
ATOM   1336  O   LEU   164       1.011   9.415  18.223  1.00  7.63
ATOM   1337  N   GLY   165       -.776  10.123  17.061  1.00  6.19
ATOM   1338  CA  GLY   165      -1.414   8.820  17.045  1.00  6.18
ATOM   1339  C   GLY   165      -2.395   8.844  18.196  1.00  6.37
ATOM   1340  O   GLY   165      -2.083   8.388  19.296  1.00  7.83
ATOM   1341  N   TRP   166      -3.585   9.379  17.953  1.00  6.29
ATOM   1342  CA  TRP   166      -4.551   9.480  19.030  1.00  5.70
ATOM   1343  CB  TRP   166      -4.478  10.871  19.668  1.00  6.48
ATOM   1344  CG  TRP   166      -4.678  12.017  18.714  1.00  6.69
ATOM   1345  CD2 TRP   166      -5.810  12.894  18.662  1.00  7.43
ATOM   1346  CE2 TRP   166      -5.560  13.844  17.647  1.00  7.37
ATOM   1347  CE3 TRP   166      -7.008  12.972  19.382  1.00  8.13
ATOM   1348  CD1 TRP   166      -3.809  12.459  17.749  1.00  6.77
ATOM   1349  NE1 TRP   166      -4.333  13.560  17.106  1.00  7.33
ATOM   1350  CZ2 TRP   166      -6.470  14.860  17.335  1.00  8.24
ATOM   1351  CZ3 TRP   166      -7.906  13.978  19.076  1.00  9.49
ATOM   1352  CH2 TRP   166      -7.635  14.909  18.061  1.00  7.95
ATOM   1353  C   TRP   166      -5.981   9.199  18.623  1.00  6.23
ATOM   1354  O   TRP   166      -6.417   9.577  17.540  1.00  6.09
ATOM   1355  N   LEU   167      -6.696   8.551  19.540  1.00  6.05
ATOM   1356  CA  LEU   167      -8.096   8.162  19.375  1.00  5.64
ATOM   1357  CB  LEU   167      -8.304   6.764  19.983  1.00  7.55
ATOM   1358  CG  LEU   167      -9.738   6.282  20.204  1.00  5.89
ATOM   1359  CD1 LEU   167     -10.367   5.868  18.866  1.00  7.30
ATOM   1360  CD2 LEU   167      -9.721   5.083  21.161  1.00  7.75
ATOM   1361  C   LEU   167      -9.040   9.137  20.079  1.00  6.64
ATOM   1362  O   LEU   167      -8.810   9.489  21.221  1.00  5.65
ATOM   1363  N   LEU   168     -10.083   9.592  19.382  1.00  6.50
ATOM   1364  CA  LEU   168     -11.084  10.455  20.008  1.00  6.91
ATOM   1365  CB  LEU   168     -10.942  11.932  19.589  1.00  6.72
ATOM   1366  CG  LEU   168     -11.538  12.387  18.254  1.00  7.53
ATOM   1367  CD1 LEU   168     -11.718  13.919  18.250  1.00  7.88
ATOM   1368  CD2 LEU   168     -10.617  11.938  17.109  1.00  6.62
ATOM   1369  C   LEU   168     -12.456   9.932  19.588  1.00  7.51
ATOM   1370  O   LEU   168     -12.584   9.249  18.567  1.00  7.30
ATOM   1371  N   LEU   169     -13.470  10.256  20.385  1.00  7.98
ATOM   1372  CA  LEU   169     -14.842   9.848  20.120  1.00  7.63
ATOM   1373  CB  LEU   169     -15.609   9.677  21.432  1.00  8.92
ATOM   1374  CG  LEU   169     -15.047   8.691  22.452  1.00  9.76
ATOM   1375  CD1 LEU   169     -15.922   8.663  23.708  1.00 11.14
ATOM   1376  CD2 LEU   169     -14.966   7.326  21.814  1.00 10.60
ATOM   1377  C   LEU   169     -15.556  10.930  19.320  1.00  7.91
ATOM   1378  O   LEU   169     -15.186  12.110  19.379  1.00  7.75
ATOM   1379  N   ALA   170     -16.596  10.517  18.600  1.00  7.99
ATOM   1380  CA  ALA   170     -17.422  11.437  17.815  1.00  8.92
ATOM   1381  CB  ALA   170     -18.548  10.662  17.132  1.00  9.49
ATOM   1382  C   ALA   170     -18.013  12.496  18.754  1.00  9.51
ATOM   1383  O   ALA   170     -18.186  13.663  18.384  1.00  8.74
ATOM   1384  N   GLU   171     -18.320  12.089  19.981  1.00  9.48
ATOM   1385  CA  GLU   171     -18.890  13.021  20.947  1.00 11.75
ATOM   1386  CB  GLU   171     -19.316  12.243  22.188  1.00 14.74
ATOM   1387  CG  GLU   171     -20.362  11.216  21.807  1.00 20.13
ATOM   1388  CD  GLU   171     -20.456  10.079  22.776  1.00 23.18
ATOM   1389  OE1 GLU   171     -20.781  10.351  23.952  1.00 26.11
ATOM   1390  OE2 GLU   171     -20.223   8.914  22.361  1.00 24.75
ATOM   1391  C   GLU   171     -17.935  14.159  21.292  1.00 11.31
ATOM   1392  O   GLU   171     -18.372  15.302  21.514  1.00 10.48
ATOM   1393  N   LEU   172     -16.633  13.872  21.327  1.00  9.49
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ATOM	1394	CA	LEU	172	-15.689	14.940	21.611	1.00	9.10
ATOM	1395	CB	LEU	172	-14.291	14.398	21.908	1.00	9.07
ATOM	1396	CG	LEU	172	-13.233	15.501	22.096	1.00	8.17
ATOM	1397	CD1	LEU	172	-13.584	16.377	23.295	1.00	9.36
ATOM	1398	CD2	LEU	172	-11.853	14.877	22.291	1.00	10.07
ATOM	1399	C	LEU	172	-15.648	15.873	20.412	1.00	8.59
ATOM	1400	O	LEU	172	-15.556	17.084	20.571	1.00	8.59
ATOM	1401	N	TRP	173	-15.724	15.318	19.204	1.00	9.64
ATOM	1402	CA	TRP	173	-15.723	16.193	18.040	1.00	9.87
ATOM	1403	CB	TRP	173	-15.753	15.394	16.730	1.00	10.77
ATOM	1404	CG	TRP	173	-15.684	16.295	15.523	1.00	11.83
ATOM	1405	CD2	TRP	173	-14.687	17.288	15.251	1.00	13.12
ATOM	1406	CE2	TRP	173	-15.049	17.921	14.038	1.00	13.92
ATOM	1407	CE3	TRP	173	-13.521	17.713	15.920	1.00	14.97
ATOM	1408	CD1	TRP	173	-16.584	16.359	14.487	1.00	12.95
ATOM	1409	NE1	TRP	173	-16.205	17.335	13.595	1.00	13.51
ATOM	1410	CZ2	TRP	173	-14.285	18.967	13.473	1.00	15.03
ATOM	1411	CZ3	TRP	173	-12.758	18.761	15.356	1.00	16.31
ATOM	1412	CH2	TRP	173	-13.155	19.369	14.140	1.00	15.65
ATOM	1413	C	TRP	173	-16.946	17.120	18.111	1.00	9.93
ATOM	1414	O	TRP	173	-16.887	18.270	17.680	1.00	10.30
ATOM	1415	N	ALA	174	-18.054	16.627	18.664	1.00	10.03
ATOM	1416	CA	ALA	174	-19.263	17.447	18.757	1.00	10.46
ATOM	1417	CB	ALA	174	-20.402	16.631	19.330	1.00	11.30
ATOM	1418	C	ALA	174	-19.009	18.663	19.628	1.00	11.04
ATOM	1419	O	ALA	174	-19.539	19.746	19.383	1.00	11.50
ATOM	1420	N	GLU	175	-18.175	18.470	20.639	1.00	10.78
ATOM	1421	CA	GLU	175	-17.813	19.515	21.590	1.00	11.03
ATOM	1422	CB	GLU	175	-17.271	18.854	22.861	1.00	12.11
ATOM	1423	CG	GLU	175	-16.767	19.808	23.921	1.00	12.43
ATOM	1424	CD	GLU	175	-16.196	19.087	25.151	1.00	11.96
ATOM	1425	OE1	GLU	175	-16.424	17.871	25.304	1.00	13.08
ATOM	1426	OE2	GLU	175	-15.532	19.744	25.987	1.00	14.26
ATOM	1427	C	GLU	175	-16.757	20.487	21.051	1.00	11.16
ATOM	1428	O	GLU	175	-16.816	21.687	21.305	1.00	10.89
ATOM	1429	N	LEU	176	-15.783	19.963	20.315	1.00	10.58
ATOM	1430	CA	LEU	176	-14.711	20.805	19.801	1.00	10.51
ATOM	1431	CB	LEU	176	-13.431	19.986	19.617	1.00	10.90
ATOM	1432	CG	LEU	176	-12.897	19.272	20.863	1.00	10.97
ATOM	1433	CD1	LEU	176	-11.568	18.603	20.549	1.00	10.70
ATOM	1434	CD2	LEU	176	-12.688	20.273	21.984	1.00	11.94
ATOM	1435	C	LEU	176	-14.995	21.567	18.505	1.00	10.59
ATOM	1436	O	LEU	176	-14.534	22.694	18.337	1.00	11.35
ATOM	1437	N	GLU	177	-15.738	20.953	17.596	1.00	12.21
ATOM	1438	CA	GLU	177	-16.027	21.565	16.297	1.00	13.68
ATOM	1439	CB	GLU	177	-16.968	20.656	15.498	1.00	14.88
ATOM	1440	CG	GLU	177	-17.120	21.038	14.015	1.00	18.01
ATOM	1441	CD	GLU	177	-17.797	19.941	13.219	1.00	20.31
ATOM	1442	OE1	GLU	177	-18.919	19.551	13.606	1.00	22.24
ATOM	1443	OE2	GLU	177	-17.215	19.444	12.213	1.00	23.26
ATOM	1444	C	GLU	177	-16.571	23.001	16.302	1.00	13.91
ATOM	1445	O	GLU	177	-16.095	23.830	15.515	1.00	14.86
ATOM	1446	N	PRO	178	-17.562	23.314	17.169	1.00	13.76
ATOM	1447	CD	PRO	178	-18.330	22.412	18.052	1.00	14.27
ATOM	1448	CA	PRO	178	-18.123	24.679	17.214	1.00	14.46
ATOM	1449	CB	PRO	178	-19.248	24.574	18.247	1.00	14.77
ATOM	1450	CG	PRO	178	-19.657	23.145	18.191	1.00	15.05
ATOM	1451	C	PRO	178	-17.150	25.798	17.598	1.00	14.28
ATOM	1452	O	PRO	178	-17.407	26.976	17.325	1.00	15.76
ATOM	1453	N	LYS	179	-16.045	25.451	18.247	1.00	13.18

ATOM	1454	CA	LYS	179	-15.089	26.460	18.671	1.00	12.26
ATOM	1455	CB	LYS	179	-15.057	26.527	20.204	1.00	11.39
ATOM	1456	CG	LYS	179	-14.794	25.180	20.885	1.00	11.14
ATOM	1457	CD	LYS	179	-14.642	25.347	22.395	1.00	11.42
ATOM	1458	CE	LYS	179	-14.269	24.045	23.078	1.00	12.19
ATOM	1459	NZ	LYS	179	-14.067	24.198	24.561	1.00	12.33
ATOM	1460	C	LYS	179	-13.690	26.187	18.126	1.00	11.16
ATOM	1461	O	LYS	179	-12.718	26.753	18.609	1.00	11.33
ATOM	1462	N	TRP	180	-13.590	25.336	17.107	1.00	10.55
ATOM	1463	CA	TRP	180	-12.280	24.992	16.538	1.00	10.74
ATOM	1464	CB	TRP	180	-12.453	24.136	15.279	1.00	11.47
ATOM	1465	CG	TRP	180	-11.197	23.430	14.833	1.00	11.48
ATOM	1466	CD2	TRP	180	-10.567	22.308	15.472	1.00	12.54
ATOM	1467	CE2	TRP	180	-9.429	21.970	14.696	1.00	11.69
ATOM	1468	CE3	TRP	180	-10.850	21.559	16.622	1.00	12.66
ATOM	1469	CD1	TRP	180	-10.435	23.714	13.727	1.00	13.11
ATOM	1470	NE1	TRP	180	-9.380	22.843	13.642	1.00	12.13
ATOM	1471	CZ2	TRP	180	-8.575	20.916	15.035	1.00	11.93
ATOM	1472	CZ3	TRP	180	-10.003	20.506	16.964	1.00	12.48
ATOM	1473	CH2	TRP	180	-8.878	20.194	16.171	1.00	12.65
ATOM	1474	C	TRP	180	-11.472	26.259	16.247	1.00	11.00
ATOM	1475	O	TRP	180	-11.973	27.222	15.671	1.00	12.29
ATOM	1476	N	PRO	181	-10.188	26.262	16.622	1.00	10.67
ATOM	1477	CD	PRO	181	-9.405	25.175	17.241	1.00	10.18
ATOM	1478	CA	PRO	181	-9.352	27.445	16.405	1.00	11.47
ATOM	1479	CB	PRO	181	-8.202	27.204	17.370	1.00	11.31
ATOM	1480	CG	PRO	181	-7.987	25.752	17.241	1.00	9.99
ATOM	1481	C	PRO	181	-8.869	27.705	14.991	1.00	12.08
ATOM	1482	O	PRO	181	-8.912	26.817	14.129	1.00	12.61
ATOM	1483	N	LYS	182	-8.400	28.933	14.769	1.00	12.48
ATOM	1484	CA	LYS	182	-7.864	29.323	13.469	1.00	13.11
ATOM	1485	CB	LYS	182	-7.713	30.848	13.368	1.00	14.84
ATOM	1486	CG	LYS	182	-9.010	31.650	13.293	1.00	17.86
ATOM	1487	CD	LYS	182	-8.694	33.145	13.121	1.00	20.26
ATOM	1488	CE	LYS	182	-9.926	34.001	12.826	1.00	21.82
ATOM	1489	NZ	LYS	182	-9.533	35.351	12.248	1.00	24.47
ATOM	1490	C	LYS	182	-6.480	28.702	13.248	1.00	11.97
ATOM	1491	O	LYS	182	-6.082	28.455	12.106	1.00	11.20
ATOM	1492	N	ALA	183	-5.747	28.477	14.346	1.00	11.97
ATOM	1493	CA	ALA	183	-4.395	27.918	14.274	1.00	11.07
ATOM	1494	CB	ALA	183	-3.412	28.996	13.797	1.00	11.37
ATOM	1495	C	ALA	183	-3.899	27.350	15.601	1.00	11.64
ATOM	1496	O	ALA	183	-4.435	27.670	16.660	1.00	11.39
ATOM	1497	N	PHE	184	-2.849	26.533	15.522	1.00	10.19
ATOM	1498	CA	PHE	184	-2.229	25.898	16.697	1.00	10.77
ATOM	1499	CB	PHE	184	-1.630	26.970	17.613	1.00	12.20
ATOM	1500	CG	PHE	184	-.700	27.900	16.904	1.00	14.31
ATOM	1501	CD1	PHE	184	-1.086	29.197	16.603	1.00	15.38
ATOM	1502	CD2	PHE	184	.549	27.456	16.494	1.00	14.51
ATOM	1503	CE1	PHE	184	-.243	30.043	15.899	1.00	16.06
ATOM	1504	CE2	PHE	184	1.408	28.294	15.787	1.00	16.55
ATOM	1505	CZ	PHE	184	1.010	29.589	15.490	1.00	15.24
ATOM	1506	C	PHE	184	-3.245	25.057	17.455	1.00	10.59
ATOM	1507	O	PHE	184	-3.380	25.167	18.679	1.00	10.77
ATOM	1508	N	TRP	185	-3.932	24.192	16.717	1.00	9.55
ATOM	1509	CA	TRP	185	-4.979	23.354	17.273	1.00	9.46
ATOM	1510	CB	TRP	185	-5.590	22.499	16.160	1.00	9.01
ATOM	1511	CG	TRP	185	-4.700	21.399	15.708	1.00	8.54
ATOM	1512	CD2	TRP	185	-4.571	20.094	16.305	1.00	8.81
ATOM	1513	CE2	TRP	185	-3.529	19.428	15.625	1.00	9.26

ATOM	1514	CE3	TRP	185	-5.234	19.434	17.352	1.00	9.21
ATOM	1515	CD1	TRP	185	-3.770	21.459	14.718	1.00	9.72
ATOM	1516	NE1	TRP	185	-3.056	20.283	14.664	1.00	9.76
ATOM	1517	CZ2	TRP	185	-3.128	18.133	15.956	1.00	10.42
ATOM	1518	CZ3	TRP	185	-4.834	18.151	17.685	1.00	9.99
ATOM	1519	CH2	TRP	185	-3.787	17.510	16.987	1.00	9.50
ATOM	1520	C	TRP	185	-4.608	22.457	18.450	1.00	8.98
ATOM	1521	O	TRP	185	-5.437	22.249	19.347	1.00	8.63
ATOM	1522	N	ASP	186	-3.377	21.946	18.476	1.00	9.62
ATOM	1523	CA	ASP	186	-3.007	21.049	19.561	1.00	10.08
ATOM	1524	CB	ASP	186	-1.894	20.081	19.115	1.00	11.66
ATOM	1525	CG	ASP	186	-.666	20.776	18.569	1.00	13.62
ATOM	1526	OD1	ASP	186	-.727	21.942	18.125	1.00	15.84
ATOM	1527	OD2	ASP	186	.395	20.131	18.581	1.00	16.45
ATOM	1528	C	ASP	186	-2.690	21.763	20.865	1.00	9.62
ATOM	1529	O	ASP	186	-3.012	21.257	21.923	1.00	10.27
ATOM	1530	N	ASP	187	-2.098	22.948	20.806	1.00	9.91
ATOM	1531	CA	ASP	187	-1.855	23.673	22.041	1.00	9.94
ATOM	1532	CB	ASP	187	-.842	24.794	21.811	1.00	11.52
ATOM	1533	CG	ASP	187	.585	24.282	21.772	1.00	13.05
ATOM	1534	OD1	ASP	187	.865	23.159	22.262	1.00	13.41
ATOM	1535	OD2	ASP	187	1.436	25.020	21.265	1.00	15.52
ATOM	1536	C	ASP	187	-3.198	24.226	22.540	1.00	9.36
ATOM	1537	O	ASP	187	-3.397	24.426	23.751	1.00	9.17
ATOM	1538	N	TRP	188	-4.124	24.450	21.606	1.00	9.13
ATOM	1539	CA	TRP	188	-5.463	24.937	21.950	1.00	8.30
ATOM	1540	CB	TRP	188	-6.213	25.285	20.659	1.00	8.47
ATOM	1541	CG	TRP	188	-7.659	25.637	20.835	1.00	8.72
ATOM	1542	CD2	TRP	188	-8.762	24.765	20.627	1.00	9.04
ATOM	1543	CE2	TRP	188	-9.938	25.511	20.861	1.00	9.33
ATOM	1544	CE3	TRP	188	-8.873	23.415	20.262	1.00	9.54
ATOM	1545	CD1	TRP	188	-8.187	26.852	21.189	1.00	9.43
ATOM	1546	NE1	TRP	188	-9.555	26.785	21.204	1.00	10.04
ATOM	1547	CZ2	TRP	188	-11.212	24.952	20.741	1.00	8.95
ATOM	1548	CZ3	TRP	188	-10.134	22.861	20.143	1.00	8.40
ATOM	1549	CH2	TRP	188	-11.290	23.627	20.380	1.00	9.47
ATOM	1550	C	TRP	188	-6.198	23.836	22.739	1.00	8.35
ATOM	1551	O	TRP	188	-6.875	24.108	23.731	1.00	7.67
ATOM	1552	N	MET	189	-6.042	22.588	22.307	1.00	8.44
ATOM	1553	CA	MET	189	-6.690	21.493	23.021	1.00	9.09
ATOM	1554	CB	MET	189	-6.541	20.180	22.238	1.00	10.28
ATOM	1555	CG	MET	189	-7.635	19.995	21.179	1.00	12.29
ATOM	1556	SD	MET	189	-7.489	18.471	20.283	1.00	13.38
ATOM	1557	CE	MET	189	-7.844	17.315	21.550	1.00	13.10
ATOM	1558	C	MET	189	-6.104	21.334	24.416	1.00	8.97
ATOM	1559	O	MET	189	-6.783	20.873	25.330	1.00	9.41
ATOM	1560	N	ARG	190	-4.836	21.702	24.574	1.00	8.63
ATOM	1561	CA	ARG	190	-4.164	21.581	25.861	1.00	8.08
ATOM	1562	CB	ARG	190	-2.644	21.591	25.646	1.00	7.49
ATOM	1563	CG	ARG	190	-2.180	20.366	24.855	1.00	8.47
ATOM	1564	CD	ARG	190	-.745	20.461	24.371	1.00	8.61
ATOM	1565	NE	ARG	190	-.348	19.219	23.710	1.00	10.57
ATOM	1566	CZ	ARG	190	.330	19.156	22.570	1.00	12.45
ATOM	1567	NH1	ARG	190	.705	20.264	21.933	1.00	13.52
ATOM	1568	NH2	ARG	190	.621	17.977	22.052	1.00	13.01
ATOM	1569	C	ARG	190	-4.565	22.633	26.885	1.00	8.30
ATOM	1570	O	ARG	190	-4.237	22.507	28.062	1.00	9.72
ATOM	1571	N	ARG	191	-5.289	23.654	26.445	1.00	8.88
ATOM	1572	CA	ARG	191	-5.745	24.703	27.357	1.00	8.99
ATOM	1573	CB	ARG	191	-6.239	25.919	26.569	1.00	9.50

ATOM	1574	CG	ARG	191	-5.163	26.703	25.834	1.00	11.91
ATOM	1575	CD	ARG	191	-5.813	27.786	24.963	1.00	13.38
ATOM	1576	NE	ARG	191	-4.864	28.478	24.090	1.00	15.60
ATOM	1577	CZ	ARG	191	-5.220	29.420	23.213	1.00	17.69
ATOM	1578	NH1	ARG	191	-6.499	29.776	23.084	1.00	19.05
ATOM	1579	NH2	ARG	191	-4.291	30.032	22.494	1.00	18.47
ATOM	1580	C	ARG	191	-6.883	24.147	28.207	1.00	8.91
ATOM	1581	O	ARG	191	-7.667	23.306	27.747	1.00	9.33
ATOM	1582	N	PRO	192	-7.000	24.622	29.460	1.00	10.06
ATOM	1583	CD	PRO	192	-6.158	25.632	30.130	1.00	10.86
ATOM	1584	CA	PRO	192	-8.060	24.136	30.353	1.00	10.10
ATOM	1585	CB	PRO	192	-7.783	24.878	31.664	1.00	11.29
ATOM	1586	CG	PRO	192	-7.056	26.125	31.230	1.00	10.78
ATOM	1587	C	PRO	192	-9.484	24.332	29.855	1.00	10.80
ATOM	1588	O	PRO	192	-10.369	23.529	30.165	1.00	10.48
ATOM	1589	N	GLU	193	-9.700	25.383	29.068	1.00	10.87
ATOM	1590	CA	GLU	193	-11.024	25.666	28.535	1.00	11.97
ATOM	1591	CB	GLU	193	-11.030	27.005	27.792	1.00	13.91
ATOM	1592	CG	GLU	193	-10.680	28.254	28.632	1.00	18.06
ATOM	1593	CD	GLU	193	-9.212	28.337	29.034	1.00	19.60
ATOM	1594	OE1	GLU	193	-8.371	27.769	28.317	1.00	18.58
ATOM	1595	OE2	GLU	193	-8.890	28.980	30.070	1.00	22.29
ATOM	1596	C	GLU	193	-11.464	24.547	27.588	1.00	11.21
ATOM	1597	O	GLU	193	-12.652	24.371	27.358	1.00	12.55
ATOM	1598	N	GLN	194	-10.508	23.808	27.029	1.00	10.05
ATOM	1599	CA	GLN	194	-10.837	22.690	26.154	1.00	9.30
ATOM	1600	CB	GLN	194	-9.922	22.642	24.926	1.00	9.29
ATOM	1601	CG	GLN	194	-10.342	23.560	23.768	1.00	9.28
ATOM	1602	CD	GLN	194	-10.430	25.020	24.166	1.00	10.91
ATOM	1603	OE1	GLN	194	-11.519	25.552	24.386	1.00	10.82
ATOM	1604	NE2	GLN	194	-9.281	25.674	24.269	1.00	9.37
ATOM	1605	C	GLN	194	-10.726	21.362	26.903	1.00	9.60
ATOM	1606	O	GLN	194	-11.650	20.555	26.889	1.00	8.35
ATOM	1607	N	ARG	195	-9.605	21.148	27.588	1.00	9.22
ATOM	1608	CA	ARG	195	-9.375	19.886	28.297	1.00	8.73
ATOM	1609	CB	ARG	195	-7.931	19.850	28.812	1.00	8.60
ATOM	1610	CG	ARG	195	-7.497	18.488	29.319	1.00	8.18
ATOM	1611	CD	ARG	195	-6.012	18.489	29.645	1.00	9.95
ATOM	1612	NE	ARG	195	-5.700	19.151	30.910	1.00	10.34
ATOM	1613	CZ	ARG	195	-5.780	18.559	32.100	1.00	11.50
ATOM	1614	NH1	ARG	195	-6.176	17.297	32.198	1.00	11.18
ATOM	1615	NH2	ARG	195	-5.408	19.205	33.196	1.00	12.77
ATOM	1616	C	ARG	195	-10.356	19.566	29.437	1.00	8.61
ATOM	1617	O	ARG	195	-10.715	18.408	29.650	1.00	7.85
ATOM	1618	N	LYS	196	-10.771	20.594	30.168	1.00	9.01
ATOM	1619	CA	LYS	196	-11.708	20.432	31.272	1.00	9.67
ATOM	1620	CB	LYS	196	-13.122	20.188	30.732	1.00	10.67
ATOM	1621	CG	LYS	196	-13.681	21.369	29.930	1.00	11.70
ATOM	1622	CD	LYS	196	-14.942	20.982	29.148	1.00	13.59
ATOM	1623	CE	LYS	196	-15.476	22.170	28.343	1.00	15.13
ATOM	1624	NZ	LYS	196	-16.698	21.833	27.533	1.00	16.25
ATOM	1625	C	LYS	196	-11.295	19.326	32.247	1.00	9.50
ATOM	1626	O	LYS	196	12.125	18.534	32.700	1.00	10.67
ATOM	1627	N	GLY	197	-10.031	19.291	32.547	1.00	10.07
ATOM	1628	CA	GLY	197	-9.460	18.327	33.494	1.00	9.50
ATOM	1629	C	GLY	197	-9.394	16.892	33.022	1.00	9.21
ATOM	1630	O	GLY	197	-9.054	15.991	33.799	1.00	10.00
ATOM	1631	N	ARG	198	-9.683	16.660	31.750	1.00	8.68
ATOM	1632	CA	ARG	198	-9.681	15.291	31.242	1.00	8.71
ATOM	1633	CB	ARG	198	-10.635	15.183	30.057	1.00	9.17

ATOM	1634	CG	ARG	198	-12.103	15.265	30.497	1.00	7.39
ATOM	1635	CD	ARG	198	-13.074	15.408	29.341	1.00	9.26
ATOM	1636	NE	ARG	198	-12.863	16.653	28.604	1.00	8.66
ATOM	1637	CZ	ARG	198	-13.726	17.162	27.729	1.00	9.96
ATOM	1638	NH1	ARG	198	-14.865	16.526	27.471	1.00	9.57
ATOM	1639	NH2	ARG	198	-13.462	18.323	27.135	1.00	10.00
ATOM	1640	C	ARG	198	-8.303	14.745	30.903	1.00	8.33
ATOM	1641	O	ARG	198	-7.382	15.486	30.558	1.00	9.15
ATOM	1642	N	ALA	199	-8.169	13.432	31.000	1.00	7.99
ATOM	1643	CA	ALA	199	-6.885	12.791	30.748	1.00	8.10
ATOM	1644	CB	ALA	199	-6.493	11.969	31.979	1.00	8.79
ATOM	1645	C	ALA	199	-6.894	11.891	29.526	1.00	7.20
ATOM	1646	O	ALA	199	-7.921	11.643	28.927	1.00	6.19
ATOM	1647	N	CYS	200	-5.715	11.414	29.156	1.00	7.72
ATOM	1648	CA	CYS	200	-5.585	10.481	28.042	1.00	7.71
ATOM	1649	C	CYS	200	-4.810	9.291	28.577	1.00	6.40
ATOM	1650	O	CYS	200	-4.120	9.381	29.576	1.00	7.60
ATOM	1651	CB	CYS	200	-4.726	11.018	26.913	1.00	9.36
ATOM	1652	SG	CYS	200	-5.305	12.364	25.836	1.00	13.09
ATOM	1653	N	VAL	201	-4.928	8.173	27.887	1.00	6.46
ATOM	1654	CA	VAL	201	-4.164	6.993	28.241	1.00	5.67
ATOM	1655	CB	VAL	201	-4.963	5.722	27.900	1.00	6.60
ATOM	1656	CG1	VAL	201	-4.083	4.475	28.004	1.00	7.17
ATOM	1657	CG2	VAL	201	-6.128	5.585	28.883	1.00	7.12
ATOM	1658	C	VAL	201	-2.913	7.076	27.362	1.00	6.04
ATOM	1659	O	VAL	201	-3.003	7.469	26.197	1.00	6.65
ATOM	1660	N	ARG	202	-1.744	6.775	27.926	1.00	5.80
ATOM	1661	CA	ARG	202	-.511	6.776	27.141	1.00	5.38
ATOM	1662	CB	ARG	202	.241	8.113	27.282	1.00	5.51
ATOM	1663	CG	ARG	202	.816	8.420	28.658	1.00	6.08
ATOM	1664	CD	ARG	202	2.179	7.761	28.841	1.00	7.57
ATOM	1665	NE	ARG	202	2.807	8.151	30.098	1.00	6.66
ATOM	1666	CZ	ARG	202	3.972	7.673	30.526	1.00	7.73
ATOM	1667	NH1	ARG	202	4.634	6.780	29.800	1.00	7.81
ATOM	1668	NH2	ARG	202	4.479	8.098	31.682	1.00	8.19
ATOM	1669	C	ARG	202	.326	5.574	27.592	1.00	5.50
ATOM	1670	O	ARG	202	.173	5.077	28.722	1.00	5.76
ATOM	1671	N	PRO	203	1.223	5.083	26.725	1.00	5.30
ATOM	1672	CD	PRO	203	1.384	5.387	25.287	1.00	5.92
ATOM	1673	CA	PRO	203	2.033	3.921	27.102	1.00	4.52
ATOM	1674	CB	PRO	203	2.099	3.140	25.799	1.00	5.88
ATOM	1675	CG	PRO	203	2.319	4.267	24.814	1.00	7.39
ATOM	1676	C	PRO	203	3.419	4.166	27.638	1.00	5.74
ATOM	1677	O	PRO	203	3.963	5.250	27.516	1.00	6.52
ATOM	1678	N	GLU	204	3.984	3.118	28.222	1.00	5.75
ATOM	1679	CA	GLU	204	5.347	3.162	28.724	1.00	6.03
ATOM	1680	CB	GLU	204	5.641	1.886	29.520	1.00	6.66
ATOM	1681	CG	GLU	204	7.128	1.673	29.878	1.00	7.83
ATOM	1682	CD	GLU	204	7.613	2.556	31.022	1.00	10.35
ATOM	1683	OE1	GLU	204	6.799	3.314	31.585	1.00	10.93
ATOM	1684	OE2	GLU	204	8.813	2.475	31.371	1.00	9.64
ATOM	1685	C	GLU	204	6.270	3.236	27.495	1.00	5.97
ATOM	1686	O	GLU	204	7.281	3.956	27.493	1.00	7.38
ATOM	1687	N	ILE	205	5.918	2.477	26.457	1.00	5.73
ATOM	1688	CA	ILE	205	6.702	2.451	25.225	1.00	5.30
ATOM	1689	CB	ILE	205	7.265	1.037	24.942	1.00	5.98
ATOM	1690	CG2	ILE	205	8.289	1.114	23.811	1.00	7.14
ATOM	1691	CG1	ILE	205	7.933	.471	26.205	1.00	7.73
ATOM	1692	CD1	ILE	205	8.640	-.868	25.977	1.00	9.07
ATOM	1693	C	ILE	205	5.776	2.884	24.093	1.00	5.07

ATOM	1694	O	ILE	205	4.703	2.313	23.884	1.00	5.57
ATOM	1695	N	SER	206	6.195	3.910	23.367	1.00	6.04
ATOM	1696	CA	SER	206	5.371	4.453	22.298	1.00	6.00
ATOM	1697	CB	SER	206	6.060	5.665	21.687	1.00	7.46
ATOM	1698	OG	SER	206	6.300	6.611	22.703	1.00	10.52
ATOM	1699	C	SER	206	4.979	3.485	21.196	1.00	6.11
ATOM	1700	O	SER	206	5.753	2.605	20.821	1.00	6.53
ATOM	1701	N	ARG	207	3.762	3.660	20.677	1.00	6.17
ATOM	1702	CA	ARG	207	3.272	2.807	19.592	1.00	5.85
ATOM	1703	CB	ARG	207	1.833	2.327	19.858	1.00	6.44
ATOM	1704	CG	ARG	207	1.756	.902	20.411	1.00	6.67
ATOM	1705	CD	ARG	207	2.468	.757	21.755	1.00	9.09
ATOM	1706	NE	ARG	207	2.614	-.643	22.143	1.00	7.56
ATOM	1707	CZ	ARG	207	3.040	-1.051	23.338	1.00	7.68
ATOM	1708	NH1	ARG	207	3.367	-.176	24.271	1.00	8.46
ATOM	1709	NH2	ARG	207	3.117	-2.341	23.607	1.00	7.45
ATOM	1710	C	ARG	207	3.365	3.495	18.235	1.00	6.46
ATOM	1711	O	ARG	207	2.873	2.978	17.228	1.00	7.07
ATOM	1712	N	THR	208	3.971	4.682	18.235	1.00	6.70
ATOM	1713	CA	THR	208	4.233	5.437	17.013	1.00	7.51
ATOM	1714	CB	THR	208	3.247	6.596	16.753	1.00	8.44
ATOM	1715	OG1	THR	208	3.143	7.403	17.931	1.00	8.18
ATOM	1716	CG2	THR	208	1.881	6.078	16.312	1.00	7.93
ATOM	1717	C	THR	208	5.610	6.070	17.175	1.00	8.17
ATOM	1718	O	THR	208	6.108	6.228	18.297	1.00	8.16
ATOM	1719	N	MET	209	6.230	6.399	16.043	1.00	9.09
ATOM	1720	CA	MET	209	7.528	7.066	16.004	1.00	10.34
ATOM	1721	CB	MET	209	8.686	6.061	15.887	1.00	12.35
ATOM	1722	CG	MET	209	8.824	5.392	14.522	1.00	16.54
ATOM	1723	SD	MET	209	10.392	4.509	14.275	1.00	22.10
ATOM	1724	CE	MET	209	11.431	5.829	13.991	1.00	21.41
ATOM	1725	C	MET	209	7.529	7.997	14.794	1.00	10.64
ATOM	1726	O	MET	209	6.910	7.696	13.778	1.00	10.02
ATOM	1727	N	THR	210	8.205	9.134	14.904	1.00	10.76
ATOM	1728	CA	THR	210	8.271	10.074	13.797	1.00	11.40
ATOM	1729	CB	THR	210	8.474	11.538	14.268	1.00	12.63
ATOM	1730	OG1	THR	210	9.695	11.646	15.013	1.00	14.80
ATOM	1731	CG2	THR	210	7.309	12.007	15.106	1.00	12.11
ATOM	1732	C	THR	210	9.455	9.705	12.916	1.00	12.56
ATOM	1733	O	THR	210	10.412	9.083	13.371	1.00	13.96
ATOM	1734	N	PHE	211	9.375	10.076	11.647	1.00	12.72
ATOM	1735	CA	PHE	211	10.452	9.811	10.703	1.00	14.14
ATOM	1736	CB	PHE	211	10.232	8.468	9.987	1.00	13.84
ATOM	1737	CG	PHE	211	9.012	8.423	9.111	1.00	13.43
ATOM	1738	CD1	PHE	211	8.989	9.103	7.894	1.00	14.24
ATOM	1739	CD2	PHE	211	7.909	7.671	9.482	1.00	13.54
ATOM	1740	CE1	PHE	211	7.873	9.025	7.054	1.00	14.71
ATOM	1741	CE2	PHE	211	6.792	7.585	8.657	1.00	13.20
ATOM	1742	CZ	PHE	211	6.774	8.263	7.440	1.00	13.88
ATOM	1743	C	PHE	211	10.510	10.976	9.707	1.00	16.03
ATOM	1744	O	PHE	211	9.556	11.759	9.592	1.00	16.48
ATOM	1745	N	GLY	212	11.645	11.104	9.018	1.00	18.22
ATOM	1746	CA	GLY	212	11.819	12.173	8.048	1.00	19.55
ATOM	1747	C	GLY	212	12.084	13.514	8.701	1.00	21.19
ATOM	1748	O	GLY	212	12.055	13.623	9.930	1.00	22.70
ATOM	1749	N	LEU	226	11.711	14.817	19.114	1.00	19.35
ATOM	1750	CA	LEU	226	10.746	13.749	18.829	1.00	18.08
ATOM	1751	CB	LEU	226	9.678	14.234	17.869	1.00	19.16
ATOM	1752	CG	LEU	226	8.799	15.363	18.364	1.00	19.52
ATOM	1753	CD1	LEU	226	8.055	15.939	17.176	1.00	20.46

ATOM	1754	CD2	LEU	226	7.858	14.860	19.451	1.00	19.34
ATOM	1755	C	LEU	226	11.377	12.528	18.197	1.00	17.45
ATOM	1756	O	LEU	226	10.900	11.412	18.384	1.00	15.98
ATOM	1757	N	LYS	227	12.439	12.757	17.430	1.00	16.95
ATOM	1758	CA	LYS	227	13.135	11.697	16.714	1.00	17.06
ATOM	1759	CB	LYS	227	14.255	12.291	15.836	1.00	19.90
ATOM	1760	CG	LYS	227	15.152	13.299	16.541	1.00	22.48
ATOM	1761	CD	LYS	227	15.887	14.199	15.548	1.00	25.02
ATOM	1762	CE	LYS	227	16.340	15.489	16.238	1.00	27.15
ATOM	1763	NZ	LYS	227	16.852	16.528	15.300	1.00	28.14
ATOM	1764	C	LYS	227	13.704	10.612	17.605	1.00	15.49
ATOM	1765	O	LYS	227	13.889	9.485	17.162	1.00	15.75
ATOM	1766	N	PHE	228	13.957	10.920	18.870	1.00	14.14
ATOM	1767	CA	PHE	228	14.524	9.894	19.726	1.00	12.68
ATOM	1768	CB	PHE	228	15.493	10.530	20.719	1.00	12.50
ATOM	1769	CG	PHE	228	16.577	11.323	20.055	1.00	13.21
ATOM	1770	CD1	PHE	228	16.620	12.702	20.196	1.00	13.76
ATOM	1771	CD2	PHE	228	17.537	10.693	19.257	1.00	14.18
ATOM	1772	CE1	PHE	228	17.610	13.457	19.551	1.00	14.05
ATOM	1773	CE2	PHE	228	18.536	11.447	18.601	1.00	15.24
ATOM	1774	CZ	PHE	228	18.562	12.824	18.758	1.00	14.24
ATOM	1775	C	PHE	228	13.554	8.960	20.452	1.00	11.84
ATOM	1776	O	PHE	228	13.990	8.069	21.169	1.00	11.27
ATOM	1777	N	ILE	229	12.253	9.140	20.254	1.00	11.59
ATOM	1778	CA	ILE	229	11.291	8.268	20.903	1.00	12.10
ATOM	1779	CB	ILE	229	9.843	8.815	20.746	1.00	12.75
ATOM	1780	CG2	ILE	229	8.872	7.672	20.456	1.00	14.91
ATOM	1781	CG1	ILE	229	9.413	9.511	22.038	1.00	15.39
ATOM	1782	CD1	ILE	229	10.167	10.738	22.345	1.00	14.82
ATOM	1783	C	ILE	229	11.434	6.890	20.263	1.00	11.81
ATOM	1784	O	ILE	229	11.499	6.769	19.030	1.00	13.47
ATOM	1785	N	LYS	230	11.497	5.868	21.111	1.00	11.72
ATOM	1786	CA	LYS	230	11.655	4.472	20.696	1.00	11.47
ATOM	1787	CB	LYS	230	12.312	3.678	21.835	1.00	13.57
ATOM	1788	CG	LYS	230	12.497	2.182	21.563	1.00	17.93
ATOM	1789	CD	LYS	230	12.743	1.414	22.857	1.00	21.02
ATOM	1790	CE	LYS	230	13.153	-.049	22.632	1.00	23.48
ATOM	1791	NZ	LYS	230	13.148	-.727	23.957	1.00	25.30
ATOM	1792	C	LYS	230	10.312	3.826	20.354	1.00	10.47
ATOM	1793	O	LYS	230	9.366	3.907	21.130	1.00	10.10
ATOM	1794	N	LEU	231	10.237	3.177	19.195	1.00	9.25
ATOM	1795	CA	LEU	231	9.009	2.493	18.786	1.00	8.36
ATOM	1796	CB	LEU	231	8.957	2.343	17.267	1.00	8.05
ATOM	1797	CG	LEU	231	7.640	1.784	16.710	1.00	8.82
ATOM	1798	CD1	LEU	231	6.499	2.706	17.130	1.00	9.08
ATOM	1799	CD2	LEU	231	7.705	1.684	15.189	1.00	10.58
ATOM	1800	C	LEU	231	8.971	1.089	19.406	1.00	8.32
ATOM	1801	O	LEU	231	9.938	.342	19.302	1.00	8.83
ATOM	1802	N	ASN	232	7.855	.737	20.039	1.00	7.77
ATOM	1803	CA	ASN	232	7.724	-.586	20.620	1.00	8.33
ATOM	1804	CB	ASN	232	6.377	-.741	21.324	1.00	9.26
ATOM	1805	CG	ASN	232	-6.174	-2.134	21.863	1.00	10.71
ATOM	1806	OD1	ASN	232	6.957	-2.611	22.685	1.00	12.61
ATOM	1807	ND2	ASN	232	5.134	-2.800	21.397	1.00	9.06
ATOM	1808	C	ASN	232	7.804	-1.636	19.514	1.00	9.85
ATOM	1809	O	ASN	232	7.233	-1.456	18.435	1.00	10.25
ATOM	1810	N	GLN	233	8.498	-2.739	19.766	1.00	11.27
ATOM	1811	CA	GLN	233	8.575	-3.767	18.737	1.00	12.85
ATOM	1812	CB	GLN	233	9.991	-3.843	18.137	1.00	15.53
ATOM	1813	CG	GLN	233	10.330	-2.715	17.126	1.00	17.51

ATOM	1814	CD	GLN	233	9.330	-2.605	15.963	1.00	18.99
ATOM	1815	OE1	GLN	233	8.921	-3.619	15.394	1.00	21.35
ATOM	1816	NE2	GLN	233	8.958	-1.386	15.593	1.00	20.34
ATOM	1817	C	GLN	233	8.130	-5.138	19.235	1.00	12.91
ATOM	1818	O	GLN	233	8.101	-6.099	18.463	1.00	14.11
ATOM	1819	N	GLN	234	7.779	-5.236	20.514	1.00	12.25
ATOM	1820	CA	GLN	234	7.312	-6.508	21.071	1.00	11.38
ATOM	1821	CB	GLN	234	7.859	-6.726	22.480	1.00	13.29
ATOM	1822	CG	GLN	234	7.617	-8.134	22.999	1.00	16.27
ATOM	1823	CD	GLN	234	8.041	-8.319	24.455	1.00	18.33
ATOM	1824	OE1	GLN	234	8.878	-7.573	24.994	1.00	19.56
ATOM	1825	NE2	GLN	234	7.473	-9.337	25.100	1.00	21.47
ATOM	1826	C	GLN	234	5.795	-6.469	21.138	1.00	10.19
ATOM	1827	O	GLN	234	5.234	-5.695	21.913	1.00	10.15
ATOM	1828	N	PHE	235	5.130	-7.303	20.345	1.00	8.42
ATOM	1829	CA	PHE	235	3.668	-7.313	20.327	1.00	7.06
ATOM	1830	CB	PHE	235	3.139	-8.348	19.327	1.00	7.98
ATOM	1831	CG	PHE	235	1.640	-8.317	19.169	1.00	7.26
ATOM	1832	CD1	PHE	235	1.042	-7.481	18.227	1.00	7.51
ATOM	1833	CD2	PHE	235	.822	-9.053	20.028	1.00	7.05
ATOM	1834	CE1	PHE	235	-.351	-7.372	18.149	1.00	8.20
ATOM	1835	CE2	PHE	235	-.571	-8.947	19.958	1.00	8.07
ATOM	1836	CZ	PHE	235	-1.155	-8.102	19.021	1.00	7.97
ATOM	1837	C	PHE	235	3.090	-7.643	21.695	1.00	7.14
ATOM	1838	O	PHE	235	3.433	-8.668	22.270	1.00	8.15
ATOM	1839	N	VAL	236	2.207	-6.778	22.194	1.00	6.83
ATOM	1840	CA	VAL	236	1.517	-6.984	23.463	1.00	6.96
ATOM	1841	CB	VAL	236	1.637	-5.757	24.365	1.00	7.10
ATOM	1842	CG1	VAL	236	.706	-5.912	25.552	1.00	7.60
ATOM	1843	CG2	VAL	236	3.058	-5.621	24.863	1.00	7.73
ATOM	1844	C	VAL	236	.030	-7.222	23.147	1.00	7.48
ATOM	1845	O	VAL	236	-.586	-6.431	22.441	1.00	7.47
ATOM	1846	N	PRO	237	-.553	-8.334	23.644	1.00	7.71
ATOM	1847	CD	PRO	237	.107	-9.429	24.394	1.00	7.95
ATOM	1848	CA	PRO	237	-1.966	-8.655	23.400	1.00	7.69
ATOM	1849	CB	PRO	237	-2.002	-10.170	23.599	1.00	7.77
ATOM	1850	CG	PRO	237	-1.064	-10.362	24.738	1.00	8.42
ATOM	1851	C	PRO	237	-2.900	-7.907	24.366	1.00	7.51
ATOM	1852	O	PRO	237	-3.558	-8.506	25.227	1.00	7.74
ATOM	1853	N	PHE	238	-2.943	-6.586	24.215	1.00	6.92
ATOM	1854	CA	PHE	238	-3.751	-5.743	25.078	1.00	7.31
ATOM	1855	CB	PHE	238	-3.730	-4.289	24.601	1.00	6.78
ATOM	1856	CG	PHE	238	-2.416	-3.601	24.814	1.00	5.89
ATOM	1857	CD1	PHE	238	-1.543	-3.379	23.752	1.00	6.88
ATOM	1858	CD2	PHE	238	-2.065	-3.146	26.075	1.00	6.07
ATOM	1859	CE1	PHE	238	-.334	-2.698	23.956	1.00	7.11
ATOM	1860	CE2	PHE	238	-.855	-2.468	26.287	1.00	6.17
ATOM	1861	CZ	PHE	238	.003	-2.244	25.222	1.00	6.81
ATOM	1862	C	PHE	238	-5.188	-6.171	25.238	1.00	7.51
ATOM	1863	O	PHE	238	-5.748	-6.001	26.320	1.00	7.49
ATOM	1864	N	THR	239	-5.785	-6.737	24.189	1.00	8.19
ATOM	1865	CA	THR	239	-7.188	-7.135	24.305	1.00	8.81
ATOM	1866	CB	THR	239	-7.865	-7.419	22.917	1.00	9.39
ATOM	1867	OG1	THR	239	-7.239	-8.526	22.263	1.00	10.69
ATOM	1868	CG2	THR	239	-7.783	-6.198	22.010	1.00	9.92
ATOM	1869	C	THR	239	-7.393	-8.348	25.214	1.00	9.40
ATOM	1870	O	THR	239	-8.535	-8.718	25.507	1.00	9.73
ATOM	1871	N	GLN	240	-6.289	-8.961	25.646	1.00	8.36
ATOM	1872	CA	GLN	240	-6.337	-10.117	26.531	1.00	9.38
ATOM	1873	CB	GLN	240	-5.380	-11.212	26.039	1.00	9.46

ATOM	1874	CG	GLN	240	-5.652	-11.674	24.593	1.00	10.30
ATOM	1875	CD	GLN	240	-4.797	-12.857	24.176	1.00	11.36
ATOM	1876	OE1	GLN	240	-3.724	-13.108	24.747	1.00	11.25
ATOM	1877	NE2	GLN	240	-5.262	-13.591	23.157	1.00	11.69
ATOM	1878	C	GLN	240	-5.946	-9.717	27.949	1.00	10.56
ATOM	1879	O	GLN	240	-5.957	-10.543	28.855	1.00	11.86
ATOM	1880	N	LEU	241	-5.622	-8.447	28.156	1.00	9.55
ATOM	1881	CA	LEU	241	-5.209	-8.002	29.481	1.00	10.58
ATOM	1882	CB	LEU	241	-4.011	-7.058	29.353	1.00	10.18
ATOM	1883	CG	LEU	241	-2.873	-7.609	28.478	1.00	10.24
ATOM	1884	CD1	LEU	241	-1.755	-6.584	28.395	1.00	11.45
ATOM	1885	CD2	LEU	241	-2.359	-8.915	29.057	1.00	11.48
ATOM	1886	C	LEU	241	-6.331	-7.314	30.241	1.00	10.47
ATOM	1887	O	LEU	241	-7.324	-6.874	29.650	1.00	11.60
ATOM	1888	N	ASP	242	-6.178	-7.240	31.558	1.00	11.08
ATOM	1889	CA	ASP	242	-7.162	-6.574	32.403	1.00	11.59
ATOM	1890	CB	ASP	242	-7.233	-7.244	33.776	1.00	13.20
ATOM	1891	CG	ASP	242	-8.341	-6.683	34.636	1.00	16.14
ATOM	1892	OD1	ASP	242	-8.798	-5.540	34.374	1.00	15.85
ATOM	1893	OD2	ASP	242	-8.750	-7.383	35.596	1.00	17.49
ATOM	1894	C	ASP	242	-6.683	-5.130	32.574	1.00	10.39
ATOM	1895	O	ASP	242	-5.746	-4.876	33.313	1.00	9.87
ATOM	1896	N	LEU	243	-7.344	-4.193	31.906	1.00	10.21
ATOM	1897	CA	LEU	243	-6.955	-2.790	31.967	1.00	10.80
ATOM	1898	CB	LEU	243	-7.035	-2.183	30.566	1.00	11.50
ATOM	1899	CG	LEU	243	-6.285	-2.942	29.461	1.00	10.95
ATOM	1900	CD1	LEU	243	-6.438	-2.170	28.156	1.00	13.25
ATOM	1901	CD2	LEU	243	-4.800	-3.083	29.803	1.00	10.94
ATOM	1902	C	LEU	243	-7.803	-1.957	32.927	1.00	11.86
ATOM	1903	O	LEU	243	-7.824	-.723	32.827	1.00	12.21
ATOM	1904	N	SER	244	-8.483	-2.626	33.853	1.00	12.20
ATOM	1905	CA	SER	244	-9.342	-1.956	34.822	1.00	12.38
ATOM	1906	CB	SER	244	-10.079	-2.993	35.694	1.00	12.62
ATOM	1907	OG	SER	244	-9.178	-3.692	36.529	1.00	15.34
ATOM	1908	C	SER	244	-8.541	-1.003	35.714	1.00	11.42
ATOM	1909	O	SER	244	-9.097	-.066	36.287	1.00	11.39
ATOM	1910	N	TYR	245	-7.233	-1.223	35.821	1.00	9.98
ATOM	1911	CA	TYR	245	-6.411	-.348	36.656	1.00	9.14
ATOM	1912	CB	TYR	245	-4.986	-.905	36.754	1.00	9.12
ATOM	1913	CG	TYR	245	-4.157	-.855	35.478	1.00	8.60
ATOM	1914	CD1	TYR	245	-3.259	.185	35.255	1.00	9.11
ATOM	1915	CE1	TYR	245	-2.418	.192	34.150	1.00	8.34
ATOM	1916	CD2	TYR	245	-4.201	-1.894	34.536	1.00	8.39
ATOM	1917	CE2	TYR	245	-3.362	-1.893	33.410	1.00	7.78
ATOM	1918	CZ	TYR	245	-2.463	-.840	33.234	1.00	7.76
ATOM	1919	OH	TYR	245	-1.580	-.818	32.169	1.00	7.74
ATOM	1920	C	TYR	245	-6.390	1.101	36.130	1.00	9.24
ATOM	1921	O	TYR	245	-6.030	2.028	36.864	1.00	7.76
ATOM	1922	N	LEU	246	-6.775	1.287	34.864	1.00	8.49
ATOM	1923	CA	LEU	246	-6.801	2.619	34.261	1.00	9.66
ATOM	1924	CB	LEU	246	-6.610	2.516	32.739	1.00	9.22
ATOM	1925	CG	LEU	246	-5.193	2.087	32.319	1.00	7.78
ATOM	1926	CD1	LEU	246	-5.190	1.747	30.849	1.00	8.41
ATOM	1927	CD2	LEU	246	-4.171	3.178	32.615	1.00	8.37
ATOM	1928	C	LEU	246	-8.059	3.431	34.585	1.00	10.77
ATOM	1929	O	LEU	246	-8.112	4.626	34.302	1.00	11.03
ATOM	1930	N	GLN	247	-9.074	2.798	35.170	1.00	12.23
ATOM	1931	CA	GLN	247	-10.280	3.545	35.556	1.00	14.23
ATOM	1932	CB	GLN	247	-11.272	2.614	36.233	1.00	17.04
ATOM	1933	CG	GLN	247	-11.518	1.315	35.465	1.00	21.01

ATOM	1934	CD	GLN	247	-12.645	.516	36.073	1.00	23.35
ATOM	1935	OE1	GLN	247	-12.530	-.705	36.277	1.00	24.79
ATOM	1936	NE2	GLN	247	-13.746	1.194	36.372	1.00	25.45
ATOM	1937	C	GLN	247	-9.853	4.631	36.537	1.00	13.74
ATOM	1938	O	GLN	247	-9.014	4.379	37.408	1.00	12.95
ATOM	1939	N	GLN	248	-10.419	5.831	36.427	1.00	14.43
ATOM	1940	CA	GLN	248	-10.008	6.923	37.312	1.00	14.73
ATOM	1941	CB	GLN	248	-10.867	8.181	37.087	1.00	16.24
ATOM	1942	CG	GLN	248	-10.328	9.413	37.824	1.00	17.20
ATOM	1943	CD	GLN	248	-11.121	10.687	37.558	1.00	18.70
ATOM	1944	OE1	GLN	248	-12.328	10.754	37.817	1.00	20.13
ATOM	1945	NE2	GLN	248	-10.441	11.709	37.055	1.00	19.80
ATOM	1946	C	GLN	248	-9.987	6.609	38.806	1.00	15.06
ATOM	1947	O	GLN	248	-8.996	6.888	39.479	1.00	13.80
ATOM	1948	N	GLU	249	-11.072	6.041	39.333	1.00	15.69
ATOM	1949	CA	GLU	249	-11.141	5.745	40.764	1.00	17.06
ATOM	1950	CB	GLU	249	-12.516	5.119	41.124	1.00	19.21
ATOM	1951	CG	GLU	249	-12.865	3.803	40.405	1.00	23.09
ATOM	1952	CD	GLU	249	-13.573	3.991	39.055	1.00	24.76
ATOM	1953	OE1	GLU	249	-13.365	5.027	38.372	1.00	25.82
ATOM	1954	OE2	GLU	249	-14.343	3.077	38.659	1.00	25.35
ATOM	1955	C	GLU	249	-9.972	4.857	41.235	1.00	16.69
ATOM	1956	O	GLU	249	-9.277	5.191	42.217	1.00	18.11
ATOM	1957	N	ALA	250	-9.721	3.761	40.510	1.00	15.07
ATOM	1958	CA	ALA	250	-8.628	2.837	40.843	1.00	13.16
ATOM	1959	CB	ALA	250	-8.718	1.597	39.957	1.00	13.08
ATOM	1960	C	ALA	250	-7.244	3.490	40.677	1.00	12.05
ATOM	1961	O	ALA	250	-6.411	3.453	41.580	1.00	11.97
ATOM	1962	N	TYR	251	-7.018	4.097	39.522	1.00	11.09
ATOM	1963	CA	TYR	251	-5.745	4.734	39.221	1.00	10.15
ATOM	1964	CB	TYR	251	-5.803	5.374	37.839	1.00	9.05
ATOM	1965	CG	TYR	251	-4.442	5.620	37.237	1.00	7.87
ATOM	1966	CD1	TYR	251	-3.794	4.616	36.517	1.00	7.43
ATOM	1967	CE1	TYR	251	-2.542	4.823	35.967	1.00	8.06
ATOM	1968	CD2	TYR	251	-3.797	6.845	37.395	1.00	8.56
ATOM	1969	CE2	TYR	251	-2.537	7.070	36.843	1.00	7.67
ATOM	1970	CZ	TYR	251	-1.921	6.050	36.131	1.00	6.73
ATOM	1971	OH	TYR	251	-.683	6.240	35.574	1.00	7.25
ATOM	1972	C	TYR	251	-5.364	5.805	40.232	1.00	10.19
ATOM	1973	O	TYR	251	-4.252	5.817	40.781	1.00	11.04
ATOM	1974	N	ASP	252	-6.295	6.715	40.473	1.00	10.65
ATOM	1975	CA	ASP	252	-6.050	7.821	41.385	1.00	12.54
ATOM	1976	CB	ASP	252	-7.209	8.811	41.309	1.00	12.14
ATOM	1977	CG	ASP	252	-7.116	9.708	40.090	1.00	14.04
ATOM	1978	OD1	ASP	252	-6.244	9.433	39.238	1.00	13.70
ATOM	1979	OD2	ASP	252	-7.906	10.686	39.988	1.00	15.01
ATOM	1980	C	ASP	252	-5.788	7.399	42.811	1.00	13.75
ATOM	1981	O	ASP	252	-5.198	8.150	43.570	1.00	16.75
ATOM	1982	N	ARG	253	-6.237	6.211	43.183	1.00	13.70
ATOM	1983	CA	ARG	253	-5.975	5.702	44.526	1.00	14.49
ATOM	1984	CB	ARG	253	-7.085	4.738	44.944	1.00	15.10
ATOM	1985	CG	ARG	253	-6.805	3.961	46.211	1.00	18.72
ATOM	1986	CD	ARG	253	-7.829	2.837	46.404	1.00	20.30
ATOM	1987	NE	ARG	253	-7.702	1.771	45.405	1.00	23.42
ATOM	1988	CZ	ARG	253	-8.695	1.389	44.594	1.00	24.21
ATOM	1989	NH1	ARG	253	-9.883	1.990	44.670	1.00	25.59
ATOM	1990	NH2	ARG	253	-8.513	.413	43.705	1.00	24.81
ATOM	1991	C	ARG	253	-4.646	4.947	44.514	1.00	13.41
ATOM	1992	O	ARG	253	-3.709	5.287	45.239	1.00	12.91
ATOM	1993	N	ASP	254	-4.565	3.934	43.655	1.00	12.65

ATOM	1994	CA	ASP	254	-3.390	3.091	43.575	1.00	13.21
ATOM	1995	CB	ASP	254	-3.736	1.827	42.785	1.00	14.52
ATOM	1996	CG	ASP	254	-4.770	.961	43.498	1.00	16.38
ATOM	1997	OD1	ASP	254	-4.915	1.104	44.735	1.00	17.53
ATOM	1998	OD2	ASP	254	-5.425	.113	42.840	1.00	17.71
ATOM	1999	C	ASP	254	-2.122	3.732	43.013	1.00	12.77
ATOM	2000	O	ASP	254	-1.047	3.604	43.594	1.00	12.43
ATOM	2001	N	PHE	255	-2.211	4.435	41.893	1.00	12.85
ATOM	2002	CA	PHE	255	-.984	5.024	41.384	1.00	13.39
ATOM	2003	CB	PHE	255	-1.174	5.567	39.975	1.00	13.16
ATOM	2004	CG	PHE	255	.117	5.929	39.305	1.00	12.76
ATOM	2005	CD1	PHE	255	1.014	4.934	38.899	1.00	12.29
ATOM	2006	CD2	PHE	255	.456	7.257	39.108	1.00	12.12
ATOM	2007	CE1	PHE	255	2.237	5.277	38.300	1.00	12.03
ATOM	2008	CE2	PHE	255	1.666	7.603	38.514	1.00	11.00
ATOM	2009	CZ	PHE	255	2.560	6.608	38.108	1.00	11.69
ATOM	2010	C	PHE	255	-.452	6.134	42.297	1.00	13.94
ATOM	2011	O	PHE	255	.756	6.263	42.498	1.00	13.31
ATOM	2012	N	LEU	256	-1.339	6.940	42.857	1.00	14.07
ATOM	2013	CA	LEU	256	-.905	8.004	43.758	1.00	14.67
ATOM	2014	CB	LEU	256	-2.059	8.970	44.024	1.00	16.24
ATOM	2015	CG	LEU	256	-2.244	9.981	42.892	1.00	18.03
ATOM	2016	CD1	LEU	256	-3.720	10.334	42.738	1.00	20.23
ATOM	2017	CD2	LEU	256	-1.362	11.219	43.166	1.00	18.62
ATOM	2018	C	LEU	256	-.344	7.477	45.075	1.00	14.66
ATOM	2019	O	LEU	256	.620	8.028	45.613	1.00	14.59
ATOM	2020	N	ALA	257	-.945	6.416	45.610	1.00	14.23
ATOM	2021	CA	ALA	257	-.422	5.846	46.851	1.00	14.35
ATOM	2022	CB	ALA	257	-1.357	4.745	47.394	1.00	14.49
ATOM	2023	C	ALA	257	.955	5.270	46.535	1.00	14.45
ATOM	2024	O	ALA	257	1.855	5.275	47.389	1.00	14.66
ATOM	2025	N	ARG	258	1.125	4.795	45.300	1.00	14.21
ATOM	2026	CA	ARG	258	2.394	4.233	44.873	1.00	14.05
ATOM	2027	CB	ARG	258	2.243	3.583	43.497	1.00	16.01
ATOM	2028	CG	ARG	258	3.527	3.046	42.934	1.00	17.99
ATOM	2029	CD	ARG	258	3.325	2.404	41.553	1.00	17.98
ATOM	2030	NE	ARG	258	4.400	1.469	41.299	1.00	19.00
ATOM	2031	CZ	ARG	258	4.319	.140	41.404	1.00	19.22
ATOM	2032	NH1	ARG	258	3.191	-.474	41.751	1.00	19.37
ATOM	2033	NH2	ARG	258	5.406	-.581	41.178	1.00	20.16
ATOM	2034	C	ARG	258	3.458	5.318	44.810	1.00	13.68
ATOM	2035	O	ARG	258	4.569	5.139	45.304	1.00	13.64
ATOM	2036	N	VAL	259	3.110	6.452	44.199	1.00	12.99
ATOM	2037	CA	VAL	259	4.045	7.564	44.050	1.00	12.44
ATOM	2038	CB	VAL	259	3.421	8.674	43.153	1.00	12.45
ATOM	2039	CG1	VAL	259	4.284	9.949	43.163	1.00	11.57
ATOM	2040	CG2	VAL	259	3.251	8.143	41.742	1.00	12.65
ATOM	2041	C	VAL	259	4.452	8.163	45.390	1.00	12.09
ATOM	2042	O	VAL	259	5.641	8.368	45.663	1.00	12.17
ATOM	2043	N	TYR	260	3.472	8.423	46.243	1.00	11.89
ATOM	2044	CA	TYR	260	3.783	9.024	47.516	1.00	12.61
ATOM	2045	CB	TYR	260	2.615	9.891	47.967	1.00	12.61
ATOM	2046	CG	TYR	260	2.535	11.143	47.096	1.00	10.89
ATOM	2047	CD1	TYR	260	1.584	11.247	46.080	1.00	11.47
ATOM	2048	CE1	TYR	260	1.585	12.318	45.192	1.00	10.83
ATOM	2049	CD2	TYR	260	3.492	12.160	47.210	1.00	12.31
ATOM	2050	CE2	TYR	260	3.501	13.243	46.322	1.00	11.18
ATOM	2051	CZ	TYR	260	2.536	13.307	45.314	1.00	10.99
ATOM	2052	OH	TYR	260	2.510	14.379	44.438	1.00	11.04
ATOM	2053	C	TYR	260	4.242	8.061	48.594	1.00	13.66

ATOM	2054	O	TYR	260	4.712	8.501	49.644	1.00	15.16
ATOM	2055	N	GLY	261	4.118	6.765	48.320	1.00	13.77
ATOM	2056	CA	GLY	261	4.581	5.748	49.246	1.00	15.30
ATOM	2057	C	GLY	261	6.054	5.498	48.954	1.00	16.23
ATOM	2058	O	GLY	261	6.799	4.984	49.801	1.00	17.28
ATOM	2059	N	ALA	262	6.494	5.850	47.748	1.00	16.56
ATOM	2060	CA	ALA	262	7.890	5.658	47.376	1.00	16.67
ATOM	2061	CB	ALA	262	8.070	5.935	45.895	1.00	16.61
ATOM	2062	C	ALA	262	8.825	6.553	48.198	1.00	17.37
ATOM	2063	O	ALA	262	8.483	7.689	48.558	1.00	18.16
ATOM	2064	N	PRO	263	10.029	6.060	48.510	1.00	17.02
ATOM	2065	CD	PRO	263	10.633	4.737	48.301	1.00	17.75
ATOM	2066	CA	PRO	263	10.924	6.910	49.287	1.00	17.41
ATOM	2067	CB	PRO	263	12.083	5.965	49.610	1.00	17.18
ATOM	2068	CG	PRO	263	12.085	5.039	48.464	1.00	17.96
ATOM	2069	C	PRO	263	11.354	8.134	48.479	1.00	17.64
ATOM	2070	O	PRO	263	11.442	8.080	47.248	1.00	16.10
ATOM	2071	N	GLN	264	11.594	9.242	49.168	1.00	17.63
ATOM	2072	CA	GLN	264	12.033	10.476	48.536	1.00	18.22
ATOM	2073	CB	GLN	264	11.509	11.675	49.328	1.00	19.03
ATOM	2074	CG	GLN	264	11.742	13.037	48.694	1.00	21.15
ATOM	2075	CD	GLN	264	10.908	14.143	49.362	1.00	22.00
ATOM	2076	OE1	GLN	264	9.747	13.932	49.715	1.00	23.09
ATOM	2077	NE2	GLN	264	11.490	15.325	49.514	1.00	21.48
ATOM	2078	C	GLN	264	13.567	10.529	48.460	1.00	18.23
ATOM	2079	O	GLN	264	14.261	10.108	49.396	1.00	19.12
ATOM	2080	N	LEU	265	14.097	11.015	47.343	1.00	17.20
ATOM	2081	CA	LEU	265	15.544	11.159	47.158	1.00	17.32
ATOM	2082	CB	LEU	265	16.108	10.118	46.183	1.00	17.97
ATOM	2083	CG	LEU	265	16.333	8.700	46.696	1.00	18.17
ATOM	2084	CD1	LEU	265	17.250	7.934	45.750	1.00	17.13
ATOM	2085	CD2	LEU	265	16.949	8.769	48.061	1.00	19.48
ATOM	2086	C	LEU	265	15.814	12.533	46.575	1.00	17.89
ATOM	2087	O	LEU	265	15.026	13.044	45.769	1.00	17.52
ATOM	2088	N	GLN	266	16.929	13.137	46.962	1.00	18.02
ATOM	2089	CA	GLN	266	17.260	14.441	46.415	1.00	18.63
ATOM	2090	CB	GLN	266	18.404	15.098	47.193	1.00	21.28
ATOM	2091	CG	GLN	266	18.121	15.287	48.679	1.00	25.20
ATOM	2092	CD	GLN	266	16.907	16.165	48.965	1.00	27.42
ATOM	2093	OE1	GLN	266	16.049	15.806	49.792	1.00	29.84
ATOM	2094	NE2	GLN	266	16.835	17.327	48.311	1.00	28.00
ATOM	2095	C	GLN	266	17.692	14.170	44.984	1.00	18.18
ATOM	2096	O	GLN	266	18.321	13.135	44.697	1.00	16.92
ATOM	2097	N	VAL	267	17.376	15.099	44.087	1.00	17.79
ATOM	2098	CA	VAL	267	17.711	14.935	42.679	1.00	17.86
ATOM	2099	CB	VAL	267	17.271	16.170	41.856	1.00	18.15
ATOM	2100	CG1	VAL	267	18.188	17.349	42.123	1.00	17.66
ATOM	2101	CG2	VAL	267	17.234	15.815	40.378	1.00	18.62
ATOM	2102	C	VAL	267	19.181	14.630	42.390	1.00	18.27
ATOM	2103	O	VAL	267	19.485	13.835	41.490	1.00	17.25
ATOM	2104	N	GLU	268	20.096	15.256	43.130	1.00	19.57
ATOM	2105	CA	GLU	268	21.525	15.014	42.916	1.00	21.19
ATOM	2106	CB	GLU	268	22.343	15.971	43.811	1.00	23.67
ATOM	2107	CG	GLU	268	22.334	17.456	43.313	1.00	26.97
ATOM	2108	CD	GLU	268	22.020	18.518	44.392	1.00	29.06
ATOM	2109	OE1	GLU	268	22.572	18.446	45.532	1.00	30.85
ATOM	2110	OE2	GLU	268	21.212	19.455	44.104	1.00	29.84
ATOM	2111	C	GLU	268	21.867	13.535	43.171	1.00	20.79
ATOM	2112	O	GLU	268	22.707	12.962	42.469	1.00	21.09
ATOM	2113	N	LYS	269	21.197	12.910	44.144	1.00	20.31

ATOM	2114	CA	LYS	269	21.396	11.490	44.462	1.00	19.96
ATOM	2115	CB	LYS	269	20.709	11.123	45.774	1.00	21.55
ATOM	2116	CG	LYS	269	21.385	11.665	47.007	1.00	23.28
ATOM	2117	CD	LYS	269	20.702	11.069	48.243	1.00	25.80
ATOM	2118	CE	LYS	269	21.293	11.569	49.554	1.00	27.10
ATOM	2119	NZ	LYS	269	20.596	10.935	50.732	1.00	28.29
ATOM	2120	C	LYS	269	20.878	10.564	43.370	1.00	19.16
ATOM	2121	O	LYS	269	21.493	9.529	43.081	1.00	18.50
ATOM	2122	N	VAL	270	19.738	10.914	42.767	1.00	17.50
ATOM	2123	CA	VAL	270	19.215	10.104	41.667	1.00	16.58
ATOM	2124	CB	VAL	270	17.830	10.581	41.220	1.00	15.24
ATOM	2125	CG1	VAL	270	17.445	9.900	39.928	1.00	14.27
ATOM	2126	CG2	VAL	270	16.806	10.290	42.309	1.00	13.37
ATOM	2127	C	VAL	270	20.202	10.243	40.509	1.00	17.74
ATOM	2128	O	VAL	270	20.601	9.258	39.898	1.00	16.49
ATOM	2129	N	ARG	271	20.626	11.472	40.242	1.00	18.99
ATOM	2130	CA	ARG	271	21.578	11.730	39.176	1.00	22.34
ATOM	2131	CB	ARG	271	22.066	13.172	39.248	1.00	24.16
ATOM	2132	CG	ARG	271	21.279	14.102	38.423	1.00	27.59
ATOM	2133	CD	ARG	271	21.684	13.989	36.975	1.00	30.45
ATOM	2134	NE	ARG	271	22.342	15.207	36.479	1.00	33.15
ATOM	2135	CZ	ARG	271	23.600	15.565	36.742	1.00	34.26
ATOM	2136	NH1	ARG	271	24.381	14.816	37.514	1.00	35.18
ATOM	2137	NH2	ARG	271	24.091	16.670	36.186	1.00	34.66
ATOM	2138	C	ARG	271	22.797	10.825	39.236	1.00	22.58
ATOM	2139	O	ARG	271	23.156	10.182	38.254	1.00	22.93
ATOM	2140	N	THR	272	23.438	10.767	40.396	1.00	23.55
ATOM	2141	CA	THR	272	24.652	9.976	40.495	1.00	24.48
ATOM	2142	CB	THR	272	25.619	10.664	41.447	1.00	24.83
ATOM	2143	OG1	THR	272	25.024	10.744	42.742	1.00	26.19
ATOM	2144	CG2	THR	272	25.926	12.094	40.953	1.00	25.84
ATOM	2145	C	THR	272	24.445	8.505	40.852	1.00	24.82
ATOM	2146	O	THR	272	25.389	7.780	41.204	1.00	25.38
ATOM	2147	N	ASN	273	23.203	8.053	40.743	1.00	24.54
ATOM	2148	CA	ASN	273	22.877	6.650	40.997	1.00	24.29
ATOM	2149	CB	ASN	273	23.561	5.770	39.938	1.00	24.22
ATOM	2150	CG	ASN	273	22.617	4.731	39.340	1.00	23.90
ATOM	2151	OD1	ASN	273	21.392	4.864	39.437	1.00	22.46
ATOM	2152	ND2	ASN	273	23.180	3.689	38.715	1.00	23.58
ATOM	2153	C	ASN	273	23.218	6.157	42.402	1.00	24.86
ATOM	2154	O	ASN	273	23.813	5.066	42.576	1.00	24.69
ATOM	2155	N	ASP	274	22.847	6.975	43.392	1.00	24.59
ATOM	2156	CA	ASP	274	23.026	6.667	44.811	1.00	25.51
ATOM	2157	CB	ASP	274	23.004	7.937	45.659	1.00	28.07
ATOM	2158	CG	ASP	274	24.187	8.843	45.392	1.00	30.55
ATOM	2159	OD1	ASP	274	25.322	8.321	45.271	1.00	32.70
ATOM	2160	OD2	ASP	274	23.998	10.089	45.314	1.00	32.72
ATOM	2161	C	ASP	274	21.882	5.774	45.297	1.00	24.20
ATOM	2162	O	ASP	274	20.758	5.832	44.782	1.00	23.82
ATOM	2163	N	ARG	275	22.149	4.955	46.305	1.00	22.61
ATOM	2164	CA	ARG	275	21.114	4.100	46.853	1.00	21.47
ATOM	2165	CB	ARG	275	20.074	4.957	47.582	1.00	21.80
ATOM	2166	CG	ARG	275	20.672	5.904	48.643	1.00	22.74
ATOM	2167	CD	ARG	275	20.958	5.117	49.911	1.00	22.96
ATOM	2168	NE	ARG	275	19.717	4.560	50.446	1.00	23.57
ATOM	2169	CZ	ARG	275	18.840	5.242	51.172	1.00	24.01
ATOM	2170	NH1	ARG	275	19.077	6.517	51.474	1.00	24.95
ATOM	2171	NH2	ARG	275	17.692	4.668	51.531	1.00	23.94
ATOM	2172	C	ARG	275	20.408	3.269	45.788	1.00	20.42
ATOM	2173	O	ARG	275	19.181	3.339	45.663	1.00	20.52

ATOM	2174	N	LYS	276	21.157	2.462	45.049	1.00	19.61
ATOM	2175	CA	LYS	276	20.540	1.653	44.003	1.00	18.95
ATOM	2176	CB	LYS	276	21.618	1.041	43.108	1.00	19.86
ATOM	2177	CG	LYS	276	22.224	2.037	42.129	1.00	22.18
ATOM	2178	CD	LYS	276	23.302	1.396	41.241	1.00	23.87
ATOM	2179	CE	LYS	276	22.880	.002	40.754	1.00	24.91
ATOM	2180	NZ	LYS	276	21.599	.034	39.982	1.00	27.01
ATOM	2181	C	LYS	276	19.576	.567	44.489	1.00	17.85
ATOM	2182	O	LYS	276	18.845	-.025	43.686	1.00	17.51
ATOM	2183	N	GLU	277	19.577	.287	45.790	1.00	16.36
ATOM	2184	CA	GLU	277	18.669	-.707	46.348	1.00	15.30
ATOM	2185	CB	GLU	277	18.997	-.974	47.832	1.00	14.31
ATOM	2186	CG	GLU	277	18.685	.167	48.764	1.00	14.71
ATOM	2187	CD	GLU	277	19.871	1.060	49.052	1.00	14.97
ATOM	2188	OE1	GLU	277	20.802	1.146	48.217	1.00	15.81
ATOM	2189	OE2	GLU	277	19.867	1.694	50.131	1.00	17.06
ATOM	2190	C	GLU	277	17.226	-.209	46.209	1.00	15.48
ATOM	2191	O	GLU	277	16.292	-1.010	46.208	1.00	14.85
ATOM	2192	N	LEU	278	17.044	1.105	46.071	1.00	14.82
ATOM	2193	CA	LEU	278	15.695	1.657	45.925	1.00	15.11
ATOM	2194	CB	LEU	278	15.628	3.069	46.518	1.00	16.29
ATOM	2195	CG	LEU	278	16.078	3.217	47.980	1.00	16.35
ATOM	2196	CD1	LEU	278	16.088	4.692	48.356	1.00	16.47
ATOM	2197	CD2	LEU	278	15.164	2.409	48.901	1.00	17.83
ATOM	2198	C	LEU	278	15.342	1.704	44.444	1.00	15.11
ATOM	2199	O	LEU	278	15.761	2.610	43.730	1.00	15.93
ATOM	2200	N	GLY	279	14.569	.732	43.987	1.00	14.70
ATOM	2201	CA	GLY	279	14.205	.671	42.582	1.00	13.74
ATOM	2202	C	GLY	279	13.114	1.613	42.117	1.00	12.15
ATOM	2203	O	GLY	279	12.848	1.710	40.922	1.00	11.95
ATOM	2204	N	GLU	280	12.491	2.315	43.047	1.00	11.84
ATOM	2205	CA	GLU	280	11.426	3.241	42.705	1.00	11.71
ATOM	2206	CB	GLU	280	10.067	2.534	42.769	1.00	13.39
ATOM	2207	CG	GLU	280	8.853	3.431	42.520	1.00	15.08
ATOM	2208	CD	GLU	280	7.627	2.652	42.031	1.00	17.58
ATOM	2209	OE1	GLU	280	7.551	1.429	42.270	1.00	20.50
ATOM	2210	OE2	GLU	280	6.731	3.259	41.419	1.00	15.75
ATOM	2211	C	GLU	280	11.492	4.345	43.717	1.00	11.29
ATOM	2212	O	GLU	280	11.325	4.113	44.922	1.00	12.51
ATOM	2213	N	VAL	281	11.723	5.555	43.233	1.00	11.20
ATOM	2214	CA	VAL	281	11.822	6.699	44.118	1.00	11.83
ATOM	2215	CB	VAL	281	13.283	7.144	44.293	1.00	11.45
ATOM	2216	CG1	VAL	281	14.145	5.960	44.767	1.00	12.90
ATOM	2217	CG2	VAL	281	13.816	7.715	42.973	1.00	12.94
ATOM	2218	C	VAL	281	11.044	7.906	43.624	1.00	12.69
ATOM	2219	O	VAL	281	10.573	7.960	42.486	1.00	12.44
ATOM	2220	N	ARG	282	10.929	8.886	44.504	1.00	12.51
ATOM	2221	CA	ARG	282	10.239	10.115	44.193	1.00	12.53
ATOM	2222	CB	ARG	282	9.020	10.242	45.091	1.00	13.19
ATOM	2223	CG	ARG	282	8.195	11.495	44.946	1.00	15.44
ATOM	2224	CD	ARG	282	6.929	11.308	45.762	1.00	16.79
ATOM	2225	NE	ARG	282	7.242	10.647	47.031	1.00	20.22
ATOM	2226	CZ	ARG	282	7.458	11.289	48.168	1.00	20.15
ATOM	2227	NH1	ARG	282	7.388	12.601	48.201	1.00	22.17
ATOM	2228	NH2	ARG	282	7.774	10.628	49.274	1.00	20.97
ATOM	2229	C	ARG	282	11.171	11.292	44.396	1.00	13.10
ATOM	2230	O	ARG	282	11.901	11.349	45.377	1.00	12.47
ATOM	2231	N	VAL	283	11.197	12.197	43.423	1.00	11.86
ATOM	2232	CA	VAL	283	11.995	13.418	43.515	1.00	11.54
ATOM	2233	CB	VAL	283	12.877	13.642	42.280	1.00	12.01

ATOM	2234	CG1	VAL	283	13.584	14.975	42.389	1.00	14.06
ATOM	2235	CG2	VAL	283	13.926	12.539	42.177	1.00	12.87
ATOM	2236	C	VAL	283	10.929	14.503	43.581	1.00	11.59
ATOM	2237	O	VAL	283	10.093	14.606	42.692	1.00	9.76
ATOM	2238	N	GLN	284	10.944	15.273	44.662	1.00	12.51
ATOM	2239	CA	GLN	284	9.972	16.347	44.891	1.00	14.21
ATOM	2240	CB	GLN	284	9.696	16.505	46.385	1.00	17.63
ATOM	2241	CG	GLN	284	8.262	16.286	46.780	1.00	22.66
ATOM	2242	CD	GLN	284	7.866	14.841	46.620	1.00	24.13
ATOM	2243	OE1	GLN	284	8.679	13.925	46.870	1.00	27.23
ATOM	2244	NE2	GLN	284	6.623	14.602	46.226	1.00	24.16
ATOM	2245	C	GLN	284	10.378	17.716	44.381	1.00	13.23
ATOM	2246	O	GLN	284	11.510	18.165	44.591	1.00	14.80
ATOM	2247	N	TYR	285	9.468	18.373	43.677	1.00	12.07
ATOM	2248	CA	TYR	285	9.732	19.734	43.234	1.00	12.53
ATOM	2249	CB	TYR	285	9.622	19.860	41.713	1.00	10.88
ATOM	2250	CG	TYR	285	8.262	19.580	41.104	1.00	10.21
ATOM	2251	CD1	TYR	285	7.285	20.573	41.055	1.00	9.72
ATOM	2252	CE1	TYR	285	6.066	20.349	40.425	1.00	9.83
ATOM	2253	CD2	TYR	285	7.978	18.345	40.514	1.00	8.64
ATOM	2254	CE2	TYR	285	6.757	18.108	39.888	1.00	9.16
ATOM	2255	CZ	TYR	285	5.806	19.124	39.847	1.00	10.44
ATOM	2256	OH	TYR	285	4.592	18.917	39.231	1.00	10.30
ATOM	2257	C	TYR	285	8.700	20.583	43.977	1.00	13.61
ATOM	2258	O	TYR	285	7.670	20.074	44.393	1.00	14.53
ATOM	2259	N	THR	286	8.981	21.863	44.175	1.00	14.91
ATOM	2260	CA	THR	286	8.052	22.720	44.915	1.00	17.17
ATOM	2261	CB	THR	286	8.639	23.061	46.282	1.00	17.89
ATOM	2262	OG1	THR	286	9.848	23.801	46.104	1.00	20.31
ATOM	2263	CG2	THR	286	8.945	21.792	47.052	1.00	18.68
ATOM	2264	C	THR	286	7.689	24.025	44.209	1.00	18.18
ATOM	2265	O	THR	286	6.915	24.848	44.728	1.00	19.90
ATOM	2266	N	GLY	287	8.260	24.250	43.042	1.00	18.57
ATOM	2267	CA	GLY	287	7.936	25.475	42.332	1.00	17.87
ATOM	2268	C	GLY	287	8.276	25.307	40.877	1.00	17.82
ATOM	2269	O	GLY	287	8.864	24.298	40.487	1.00	17.32
ATOM	2270	N	ARG	288	7.904	26.290	40.069	1.00	16.97
ATOM	2271	CA	ARG	288	8.187	26.236	38.644	1.00	16.81
ATOM	2272	CB	ARG	288	7.711	27.535	37.969	1.00	18.22
ATOM	2273	CG	ARG	288	8.501	28.796	38.389	1.00	21.23
ATOM	2274	CD	ARG	288	7.612	29.790	39.098	1.00	24.47
ATOM	2275	NE	ARG	288	6.607	30.284	38.172	1.00	25.89
ATOM	2276	CZ	ARG	288	5.356	30.618	38.485	1.00	26.56
ATOM	2277	NH1	ARG	288	4.890	30.526	39.729	1.00	27.19
ATOM	2278	NH2	ARG	288	4.564	31.046	37.527	1.00	26.46
ATOM	2279	C	ARG	288	9.697	26.058	38.423	1.00	15.87
ATOM	2280	O	ARG	288	10.128	25.225	37.627	1.00	13.94
ATOM	2281	N	ASP	289	10.497	26.853	39.126	1.00	14.95
ATOM	2282	CA	ASP	289	11.950	26.806	38.992	1.00	15.64
ATOM	2283	CB	ASP	289	12.601	27.886	39.856	1.00	18.06
ATOM	2284	CG	ASP	289	12.341	29.302	39.329	1.00	21.44
ATOM	2285	OD1	ASP	289	11.969	29.481	38.136	1.00	23.54
ATOM	2286	OD2	ASP	289	12.528	30.248	40.119	1.00	23.97
ATOM	2287	C	ASP	289	12.565	25.449	39.326	1.00	14.59
ATOM	2288	O	ASP	289	13.415	24.949	38.570	1.00	13.99
ATOM	2289	N	SER	290	12.148	24.863	40.450	1.00	12.79
ATOM	2290	CA	SER	290	12.650	23.556	40.851	1.00	12.32
ATOM	2291	CB	SER	290	12.233	23.216	42.298	1.00	12.00
ATOM	2292	OG	SER	290	10.832	23.190	42.469	1.00	13.43
ATOM	2293	C	SER	290	12.168	22.482	39.874	1.00	11.91

ATOM	2294	O	SER	290	12.891	21.539	39.586	1.00	11.98
ATOM	2295	N	PHE	291	10.958	22.620	39.345	1.00	11.91
ATOM	2296	CA	PHE	291	10.503	21.637	38.373	1.00	11.53
ATOM	2297	CB	PHE	291	9.078	21.921	37.905	1.00	11.00
ATOM	2298	CG	PHE	291	8.688	21.090	36.728	1.00	10.94
ATOM	2299	CD1	PHE	291	8.405	19.742	36.890	1.00	11.22
ATOM	2300	CD2	PHE	291	8.719	21.620	35.444	1.00	11.46
ATOM	2301	CE1	PHE	291	8.166	18.919	35.783	1.00	11.62
ATOM	2302	CE2	PHE	291	8.481	20.816	34.335	1.00	12.99
ATOM	2303	CZ	PHE	291	8.208	19.464	34.504	1.00	10.80
ATOM	2304	C	PHE	291	11.403	21.656	37.137	1.00	12.51
ATOM	2305	O	PHE	291	11.838	20.610	36.653	1.00	11.92
ATOM	2306	N	LYS	292	11.651	22.853	36.606	1.00	13.20
ATOM	2307	CA	LYS	292	12.492	23.011	35.427	1.00	14.29
ATOM	2308	CB	LYS	292	12.567	24.487	35.037	1.00	16.18
ATOM	2309	CG	LYS	292	11.290	25.037	34.474	1.00	20.20
ATOM	2310	CD	LYS	292	11.179	24.691	33.009	1.00	22.82
ATOM	2311	CE	LYS	292	10.038	25.397	32.315	1.00	23.52
ATOM	2312	NZ	LYS	292	10.320	25.340	30.849	1.00	24.68
ATOM	2313	C	LYS	292	13.897	22.487	35.670	1.00	13.73
ATOM	2314	O	LYS	292	14.457	21.778	34.850	1.00	13.94
ATOM	2315	N	ALA	293	14.464	22.843	36.811	1.00	12.89
ATOM	2316	CA	ALA	293	15.810	22.423	37.143	1.00	13.15
ATOM	2317	CB	ALA	293	16.245	23.108	38.412	1.00	14.17
ATOM	2318	C	ALA	293	15.968	20.911	37.280	1.00	12.83
ATOM	2319	O	ALA	293	16.906	20.321	36.711	1.00	12.88
ATOM	2320	N	PHE	294	15.066	20.291	38.041	1.00	12.28
ATOM	2321	CA	PHE	294	15.121	18.852	38.276	1.00	11.38
ATOM	2322	CB	PHE	294	14.113	18.465	39.361	1.00	11.16
ATOM	2323	CG	PHE	294	14.405	19.067	40.709	1.00	12.06
ATOM	2324	CD1	PHE	294	13.497	18.936	41.754	1.00	12.07
ATOM	2325	CD2	PHE	294	15.586	19.765	40.936	1.00	12.03
ATOM	2326	CE1	PHE	294	13.753	19.489	43.006	1.00	13.09
ATOM	2327	CE2	PHE	294	15.854	20.322	42.175	1.00	13.84
ATOM	2328	CZ	PHE	294	14.942	20.188	43.212	1.00	13.35
ATOM	2329	C	PHE	294	14.864	18.055	37.003	1.00	11.80
ATOM	2330	O	PHE	294	15.500	17.029	36.758	1.00	11.26
ATOM	2331	N	ALA	295	13.922	18.529	36.192	1.00	11.26
ATOM	2332	CA	ALA	295	13.615	17.867	34.932	1.00	11.25
ATOM	2333	CB	ALA	295	12.456	18.585	34.236	1.00	11.01
ATOM	2334	C	ALA	295	14.861	17.882	34.041	1.00	12.06
ATOM	2335	O	ALA	295	15.259	16.855	33.492	1.00	11.75
ATOM	2336	N	LYS	296	15.479	19.054	33.912	1.00	12.28
ATOM	2337	CA	LYS	296	16.679	19.199	33.089	1.00	14.81
ATOM	2338	CB	LYS	296	17.147	20.673	33.100	1.00	16.42
ATOM	2339	CG	LYS	296	18.351	20.948	32.212	1.00	20.96
ATOM	2340	CD	LYS	296	18.764	22.418	32.134	1.00	22.67
ATOM	2341	CE	LYS	296	19.913	22.582	31.109	1.00	24.78
ATOM	2342	NZ	LYS	296	20.364	24.001	30.835	1.00	26.69
ATOM	2343	C	LYS	296	17.791	18.267	33.599	1.00	14.32
ATOM	2344	O	LYS	296	18.443	17.578	32.815	1.00	14.92
ATOM	2345	N	ALA	297	17.973	18.211	34.912	1.00	14.32
ATOM	2346	CA	ALA	297	19.008	17.377	35.514	1.00	13.59
ATOM	2347	CB	ALA	297	19.055	17.611	37.007	1.00	14.50
ATOM	2348	C	ALA	297	18.832	15.895	35.245	1.00	13.95
ATOM	2349	O	ALA	297	19.805	15.145	35.200	1.00	14.44
ATOM	2350	N	LEU	298	17.588	15.465	35.097	1.00	12.93
ATOM	2351	CA	LEU	298	17.327	14.052	34.852	1.00	13.11
ATOM	2352	CB	LEU	298	16.199	13.577	35.770	1.00	13.81
ATOM	2353	CG	LEU	298	16.551	13.744	37.253	1.00	14.94

ATOM	2354	CD1	LEU	298	15.558	12.966	38.102	1.00	15.51
ATOM	2355	CD2	LEU	298	17.967	13.233	37.511	1.00	15.30
ATOM	2356	C	LEU	298	17.031	13.718	33.390	1.00	13.75
ATOM	2357	O	LEU	298	16.732	12.556	33.047	1.00	14.23
ATOM	2358	N	GLY	299	17.137	14.724	32.527	1.00	13.36
ATOM	2359	CA	GLY	299	16.931	14.517	31.104	1.00	13.59
ATOM	2360	C	GLY	299	15.489	14.330	30.685	1.00	13.02
ATOM	2361	O	GLY	299	15.216	13.697	29.661	1.00	14.43
ATOM	2362	N	VAL	300	14.579	14.904	31.463	1.00	12.87
ATOM	2363	CA	VAL	300	13.132	14.842	31.239	1.00	13.74
ATOM	2364	CB	VAL	300	12.394	14.817	32.637	1.00	15.37
ATOM	2365	CG1	VAL	300	10.910	14.717	32.470	1.00	17.44
ATOM	2366	CG2	VAL	300	12.906	13.671	33.477	1.00	16.37
ATOM	2367	C	VAL	300	12.703	16.111	30.478	1.00	13.80
ATOM	2368	O	VAL	300	13.302	17.157	30.673	1.00	12.03
ATOM	2369	N	MET	301	11.670	16.026	29.631	1.00	13.91
ATOM	2370	CA	MET	301	11.170	17.214	28.910	1.00	15.48
ATOM	2371	CB	MET	301	9.974	16.857	28.018	1.00	17.75
ATOM	2372	CG	MET	301	10.279	15.931	26.828	1.00	21.51
ATOM	2373	SD	MET	301	11.377	16.564	25.550	1.00	27.48
ATOM	2374	CE	MET	301	12.449	15.225	25.365	1.00	27.24
ATOM	2375	C	MET	301	10.723	18.240	29.967	1.00	15.13
ATOM	2376	O	MET	301	9.937	17.906	30.856	1.00	13.98
ATOM	2377	N	ASP	302	11.191	19.490	29.857	1.00	14.82
ATOM	2378	CA	ASP	302	10.866	20.497	30.859	1.00	15.83
ATOM	2379	CB	ASP	302	12.142	21.154	31.379	1.00	18.03
ATOM	2380	CG	ASP	302	12.753	22.114	30.370	1.00	21.57
ATOM	2381	OD1	ASP	302	11.989	22.875	29.704	1.00	24.46
ATOM	2382	OD2	ASP	302	13.998	22.132	30.270	1.00	23.87
ATOM	2383	C	ASP	302	9.920	21.604	30.446	1.00	15.38
ATOM	2384	O	ASP	302	9.684	22.542	31.217	1.00	16.36
ATOM	2385	N	ASP	303	9.379	21.538	29.246	1.00	14.65
ATOM	2386	CA	ASP	303	8.479	22.606	28.844	1.00	14.91
ATOM	2387	CB	ASP	303	8.525	22.821	27.325	1.00	16.78
ATOM	2388	CG	ASP	303	7.974	21.657	26.557	1.00	18.74
ATOM	2389	OD1	ASP	303	8.477	20.530	26.750	1.00	20.31
ATOM	2390	OD2	ASP	303	7.027	21.863	25.758	1.00	21.02
ATOM	2391	C	ASP	303	7.075	22.273	29.318	1.00	14.46
ATOM	2392	O	ASP	303	6.729	21.103	29.515	1.00	14.20
ATOM	2393	N	LEU	304	6.274	23.307	29.518	1.00	12.16
ATOM	2394	CA	LEU	304	4.910	23.122	29.990	1.00	12.36
ATOM	2395	CB	LEU	304	4.780	23.678	31.408	1.00	13.68
ATOM	2396	CG	LEU	304	5.740	23.136	32.472	1.00	14.11
ATOM	2397	CD1	LEU	304	6.829	24.141	32.721	1.00	15.57
ATOM	2398	CD2	LEU	304	4.961	22.822	33.735	1.00	15.14
ATOM	2399	C	LEU	304	3.890	23.814	29.095	1.00	11.60
ATOM	2400	O	LEU	304	4.161	24.887	28.573	1.00	11.51
ATOM	2401	N	LYS	305	2.730	23.182	28.902	1.00	9.87
ATOM	2402	CA	LYS	305	1.663	23.782	28.104	1.00	9.38
ATOM	2403	CB	LYS	305	1.238	22.869	26.958	1.00	10.17
ATOM	2404	CG	LYS	305	2.333	22.602	25.948	1.00	10.91
ATOM	2405	CD	LYS	305	2.705	23.871	25.219	1.00	14.00
ATOM	2406	CE	LYS	305	3.586	23.537	24.041	1.00	15.48
ATOM	2407	NZ	LYS	305	3.647	24.626	23.033	1.00	18.11
ATOM	2408	C	LYS	305	.504	23.972	29.068	1.00	8.78
ATOM	2409	O	LYS	305	-.002	23.014	29.659	1.00	8.06
ATOM	2410	N	SER	306	.099	25.227	29.227	1.00	8.02
ATOM	2411	CA	SER	306	-.968	25.598	30.148	1.00	8.20
ATOM	2412	CB	SER	306	-2.335	25.096	29.664	1.00	8.12
ATOM	2413	OG	SER	306	-2.750	25.795	28.504	1.00	8.00

ATOM	2414	C	SER	306	-.658	25.075	31.550	1.00	7.91
ATOM	2415	O	SER	306	-1.548	24.670	32.304	1.00	8.44
ATOM	2416	N	GLY	307	.627	25.091	31.891	1.00	7.72
ATOM	2417	CA	GLY	307	1.063	24.664	33.209	1.00	7.55
ATOM	2418	C	GLY	307	1.233	23.165	33.382	1.00	8.04
ATOM	2419	O	GLY	307	1.646	22.703	34.451	1.00	8.43
ATOM	2420	N	VAL	308	.946	22.398	32.331	1.00	6.88
ATOM	2421	CA	VAL	308	1.051	20.945	32.427	1.00	7.61
ATOM	2422	CB	VAL	308	-.123	20.239	31.691	1.00	6.67
ATOM	2423	CG1	VAL	308	-.094	18.741	32.001	1.00	7.82
ATOM	2424	CG2	VAL	308	-1.469	20.846	32.113	1.00	8.51
ATOM	2425	C	VAL	308	2.360	20.406	31.857	1.00	7.42
ATOM	2426	O	VAL	308	2.742	20.730	30.734	1.00	6.98
ATOM	2427	N	PRO	309	3.060	19.564	32.622	1.00	8.22
ATOM	2428	CD	PRO	309	2.818	19.191	34.029	1.00	9.33
ATOM	2429	CA	PRO	309	4.319	19.018	32.118	1.00	8.38
ATOM	2430	CB	PRO	309	5.060	18.603	33.395	1.00	9.97
ATOM	2431	CG	PRO	309	3.975	18.236	34.335	1.00	11.12
ATOM	2432	C	PRO	309	4.065	17.841	31.181	1.00	8.21
ATOM	2433	O	PRO	309	3.026	17.194	31.275	1.00	8.59
ATOM	2434	N	ARG	310	5.008	17.601	30.272	1.00	8.50
ATOM	2435	CA	ARG	310	4.928	16.491	29.325	1.00	9.65
ATOM	2436	CB	ARG	310	6.221	16.401	28.509	1.00	11.60
ATOM	2437	CG	ARG	310	6.512	17.621	27.663	1.00	14.96
ATOM	2438	CD	ARG	310	5.875	17.521	26.295	1.00	16.66
ATOM	2439	NE	ARG	310	6.127	18.745	25.532	1.00	18.26
ATOM	2440	CZ	ARG	310	5.769	18.936	24.269	1.00	18.92
ATOM	2441	NH1	ARG	310	5.137	17.981	23.589	1.00	19.83
ATOM	2442	NH2	ARG	310	6.030	20.104	23.697	1.00	19.69
ATOM	2443	C	ARG	310	4.724	15.186	30.086	1.00	8.72
ATOM	2444	O	ARG	310	5.458	14.885	31.022	1.00	9.47
ATOM	2445	N	ALA	311	3.715	14.426	29.671	1.00	8.85
ATOM	2446	CA	ALA	311	3.362	13.145	30.285	1.00	8.50
ATOM	2447	CB	ALA	311	4.506	12.129	30.109	1.00	9.33
ATOM	2448	C	ALA	311	3.001	13.278	31.762	1.00	8.60
ATOM	2449	O	ALA	311	2.904	12.278	32.482	1.00	9.66
ATOM	2450	N	GLY	312	2.751	14.499	32.216	1.00	7.99
ATOM	2451	CA	GLY	312	2.424	14.673	33.615	1.00	7.73
ATOM	2452	C	GLY	312	1.023	14.241	33.996	1.00	6.86
ATOM	2453	O	GLY	312	.100	14.347	33.190	1.00	7.83
ATOM	2454	N	TYR	313	.870	13.716	35.210	1.00	6.45
ATOM	2455	CA	TYR	313	-.446	13.343	35.720	1.00	6.77
ATOM	2456	CB	TYR	313	-.680	11.833	35.653	1.00	7.19
ATOM	2457	CG	TYR	313	-2.110	11.491	36.013	1.00	6.80
ATOM	2458	CD1	TYR	313	-3.163	11.884	35.186	1.00	7.92
ATOM	2459	CE1	TYR	313	-4.485	11.614	35.518	1.00	8.49
ATOM	2460	CD2	TYR	313	-2.411	10.817	37.190	1.00	8.65
ATOM	2461	CE2	TYR	313	-3.739	10.540	37.542	1.00	8.74
ATOM	2462	CZ	TYR	313	-4.764	10.942	36.697	1.00	9.63
ATOM	2463	OH	TYR	313	-6.076	10.644	37.011	1.00	11.68
ATOM	2464	C	TYR	313	-.485	13.831	37.177	1.00	6.73
ATOM	2465	O	TYR	313	.300	13.391	38.003	1.00	7.55
ATOM	2466	N	ARG	314	-1.392	14.760	37.473	1.00	6.21
ATOM	2467	CA	ARG	314	-1.490	15.369	38.797	1.00	7.11
ATOM	2468	CB	ARG	314	-1.972	14.352	39.841	1.00	8.32
ATOM	2469	CG	ARG	314	-3.443	13.924	39.624	1.00	9.17
ATOM	2470	CD	ARG	314	-4.030	13.127	40.802	1.00	11.03
ATOM	2471	NE	ARG	314	-4.211	13.959	41.992	1.00	13.25
ATOM	2472	CZ	ARG	314	-5.285	14.713	42.228	1.00	14.77
ATOM	2473	NH1	ARG	314	-6.295	14.748	41.361	1.00	15.16

ATOM	2474	NH2	ARG	314	-5.344	15.456	43.329	1.00	16.50
ATOM	2475	C	ARG	314	-.102	15.923	39.146	1.00	7.31
ATOM	2476	O	ARG	314	.358	15.838	40.279	1.00	7.74
ATOM	2477	N	GLY	315	.539	16.509	38.133	1.00	7.10
ATOM	2478	CA	GLY	315	1.871	17.094	38.269	1.00	7.85
ATOM	2479	C	GLY	315	3.042	16.120	38.292	1.00	8.22
ATOM	2480	O	GLY	315	4.204	16.528	38.275	1.00	8.07
ATOM	2481	N	ILE	316	2.741	14.829	38.295	1.00	7.53
ATOM	2482	CA	ILE	316	3.764	13.797	38.365	1.00	7.80
ATOM	2483	CB	ILE	316	3.236	12.546	39.130	1.00	8.27
ATOM	2484	CG2	ILE	316	4.349	11.526	39.291	1.00	8.55
ATOM	2485	CG1	ILE	316	2.654	12.957	40.490	1.00	9.18
ATOM	2486	CD1	ILE	316	1.771	11.879	41.108	1.00	12.35
ATOM	2487	C	ILE	316	4.244	13.297	37.007	1.00	7.58
ATOM	2488	O	ILE	316	3.438	12.854	36.188	1.00	8.40
ATOM	2489	N	VAL	317	5.554	13.353	36.780	1.00	7.65
ATOM	2490	CA	VAL	317	6.140	12.846	35.537	1.00	7.84
ATOM	2491	CB	VAL	317	7.140	13.848	34.924	1.00	7.72
ATOM	2492	CG1	VAL	317	7.739	13.280	33.635	1.00	8.34
ATOM	2493	CG2	VAL	317	6.435	15.182	34.641	1.00	8.21
ATOM	2494	C	VAL	317	6.867	11.552	35.921	1.00	7.41
ATOM	2495	O	VAL	317	7.733	11.554	36.796	1.00	7.88
ATOM	2496	N	THR	318	6.494	10.448	35.284	1.00	7.19
ATOM	2497	CA	THR	318	7.068	9.134	35.589	1.00	7.76
ATOM	2498	CB	THR	318	5.908	8.136	35.894	1.00	7.85
ATOM	2499	OG1	THR	318	5.139	8.626	37.007	1.00	8.11
ATOM	2500	CG2	THR	318	6.438	6.757	36.239	1.00	10.40
ATOM	2501	C	THR	318	7.954	8.623	34.440	1.00	7.95
ATOM	2502	O	THR	318	7.575	8.682	33.277	1.00	8.88
ATOM	2503	N	PHE	319	9.135	8.114	34.783	1.00	8.42
ATOM	2504	CA	PHE	319	10.083	7.653	33.774	1.00	8.24
ATOM	2505	CB	PHE	319	10.765	8.886	33.136	1.00	9.20
ATOM	2506	CG	PHE	319	11.395	9.826	34.141	1.00	8.41
ATOM	2507	CD1	PHE	319	12.771	9.823	34.352	1.00	8.97
ATOM	2508	CD2	PHE	319	10.608	10.704	34.886	1.00	9.03
ATOM	2509	CE1	PHE	319	13.351	10.670	35.286	1.00	8.58
ATOM	2510	CE2	PHE	319	11.181	11.557	35.825	1.00	10.12
ATOM	2511	CZ	PHE	319	12.558	11.540	36.029	1.00	9.36
ATOM	2512	C	PHE	319	11.144	6.754	34.398	1.00	9.84
ATOM	2513	O	PHE	319	11.146	6.541	35.610	1.00	9.61
ATOM	2514	N	LEU	320	12.035	6.228	33.559	1.00	10.62
ATOM	2515	CA	LEU	320	13.137	5.397	34.032	1.00	11.88
ATOM	2516	CB	LEU	320	13.280	4.127	33.180	1.00	12.40
ATOM	2517	CG	LEU	320	13.662	2.869	33.954	1.00	13.97
ATOM	2518	CD1	LEU	320	12.508	2.516	34.883	1.00	12.93
ATOM	2519	CD2	LEU	320	13.956	1.717	33.021	1.00	13.90
ATOM	2520	C	LEU	320	14.401	6.246	33.905	1.00	11.79
ATOM	2521	O	LEU	320	14.552	7.027	32.957	1.00	11.37
ATOM	2522	N	PHE	321	15.284	6.131	34.886	1.00	11.68
ATOM	2523	CA	PHE	321	16.538	6.863	34.868	1.00	11.15
ATOM	2524	CB	PHE	321	16.477	8.093	35.782	1.00	12.23
ATOM	2525	CG	PHE	321	17.694	8.968	35.685	1.00	11.58
ATOM	2526	CD1	PHE	321	17.794	9.933	34.689	1.00	12.70
ATOM	2527	CD2	PHE	321	18.787	8.768	36.534	1.00	12.62
ATOM	2528	CE1	PHE	321	18.958	10.677	34.534	1.00	12.54
ATOM	2529	CE2	PHE	321	19.960	9.518	36.377	1.00	13.01
ATOM	2530	CZ	PHE	321	20.039	10.468	35.377	1.00	13.71
ATOM	2531	C	PHE	321	17.584	5.885	35.376	1.00	12.05
ATOM	2532	O	PHE	321	17.539	5.473	36.542	1.00	11.68
ATOM	2533	N	ARG	322	18.509	5.503	34.494	1.00	12.90

ATOM	2534	CA	ARG	322	19.565	4.554	34.838	1.00	13.90
ATOM	2535	CB	ARG	322	20.561	5.194	35.821	1.00	16.59
ATOM	2536	CG	ARG	322	21.259	6.436	35.260	1.00	19.76
ATOM	2537	CD	ARG	322	22.271	7.078	36.224	1.00	23.03
ATOM	2538	NE	ARG	322	23.507	6.300	36.289	1.00	26.42
ATOM	2539	CZ	ARG	322	24.709	6.756	35.971	1.00	26.66
ATOM	2540	NH1	ARG	322	24.874	8.016	35.557	1.00	27.93
ATOM	2541	NH2	ARG	322	25.748	5.939	36.064	1.00	28.11
ATOM	2542	C	ARG	322	18.957	3.283	35.425	1.00	13.25
ATOM	2543	O	ARG	322	19.427	2.758	36.433	1.00	12.92
ATOM	2544	N	GLY	323	17.884	2.805	34.801	1.00	12.87
ATOM	2545	CA	GLY	323	17.234	1.583	35.246	1.00	12.61
ATOM	2546	C	GLY	323	16.299	1.666	36.440	1.00	13.39
ATOM	2547	O	GLY	323	15.646	.683	36.811	1.00	15.00
ATOM	2548	N	ARG	324	16.224	2.838	37.044	1.00	12.15
ATOM	2549	CA	ARG	324	15.401	3.052	38.209	1.00	12.90
ATOM	2550	CB	ARG	324	16.212	3.827	39.247	1.00	14.63
ATOM	2551	CG	ARG	324	15.356	4.428	40.299	1.00	18.03
ATOM	2552	CD	ARG	324	16.097	4.540	41.583	1.00	18.49
ATOM	2553	NE	ARG	324	17.339	5.298	41.497	1.00	17.16
ATOM	2554	CZ	ARG	324	18.161	5.424	42.536	1.00	16.71
ATOM	2555	NH1	ARG	324	17.835	4.847	43.683	1.00	16.18
ATOM	2556	NH2	ARG	324	19.306	6.091	42.428	1.00	18.48
ATOM	2557	C	ARG	324	14.120	3.807	37.872	1.00	11.61
ATOM	2558	O	ARG	324	14.135	4.694	37.018	1.00	11.87
ATOM	2559	N	ARG	325	13.019	3.452	38.533	1.00	10.42
ATOM	2560	CA	ARG	325	11.749	4.135	38.302	1.00	9.89
ATOM	2561	CB	ARG	325	10.559	3.254	38.710	1.00	10.63
ATOM	2562	CG	ARG	325	9.187	3.948	38.577	1.00	10.33
ATOM	2563	CD	ARG	325	8.847	4.288	37.119	1.00	9.76
ATOM	2564	NE	ARG	325	8.787	3.089	36.297	1.00	9.59
ATOM	2565	CZ	ARG	325	8.818	3.092	34.967	1.00	9.87
ATOM	2566	NH1	ARG	325	8.906	4.248	34.306	1.00	10.94
ATOM	2567	NH2	ARG	325	8.786	1.937	34.310	1.00	11.45
ATOM	2568	C	ARG	325	11.734	5.421	39.124	1.00	10.27
ATOM	2569	O	ARG	325	11.948	5.394	40.342	1.00	10.53
ATOM	2570	N	VAL	326	11.492	6.547	38.459	1.00	8.99
ATOM	2571	CA	VAL	326	11.471	7.833	39.138	1.00	9.19
ATOM	2572	CB	VAL	326	12.632	8.728	38.654	1.00	9.11
ATOM	2573	CG1	VAL	326	12.617	10.084	39.408	1.00	9.19
ATOM	2574	CG2	VAL	326	13.958	7.997	38.843	1.00	10.43
ATOM	2575	C	VAL	326	10.177	8.580	38.888	1.00	9.13
ATOM	2576	O	VAL	326	9.679	8.617	37.765	1.00	9.48
ATOM	2577	N	HIS	327	9.631	9.162	39.951	1.00	9.21
ATOM	2578	CA	HIS	327	8.424	9.966	39.840	1.00	8.57
ATOM	2579	CB	HIS	327	7.350	9.453	40.792	1.00	9.50
ATOM	2580	CG	HIS	327	6.983	8.022	40.569	1.00	9.27
ATOM	2581	CD2	HIS	327	7.205	6.919	41.323	1.00	10.69
ATOM	2582	ND1	HIS	327	6.260	7.599	39.471	1.00	9.96
ATOM	2583	CE1	HIS	327	6.047	6.297	39.564	1.00	10.92
ATOM	2584	NE2	HIS	327	6.611	5.860	40.679	1.00	10.70
ATOM	2585	C	HIS	327	-8.817	11.389	40.248	1.00	9.26
ATOM	2586	O	HIS	327	9.096	11.631	41.412	1.00	9.67
ATOM	2587	N	LEU	328	8.869	12.311	39.291	1.00	8.88
ATOM	2588	CA	LEU	328	9.178	13.717	39.578	1.00	9.71
ATOM	2589	CB	LEU	328	9.717	14.398	38.318	1.00	9.46
ATOM	2590	CG	LEU	328	10.027	15.891	38.438	1.00	9.81
ATOM	2591	CD1	LEU	328	10.913	16.130	39.650	1.00	10.25
ATOM	2592	CD2	LEU	328	10.682	16.392	37.153	1.00	11.23
ATOM	2593	C	LEU	328	7.800	14.256	39.972	1.00	9.56

ATOM	2594	O	LEU	328	6.911	14.418	39.123	1.00	9.65
ATOM	2595	N	ALA	329	7.642	14.566	41.253	1.00	9.10
ATOM	2596	CA	ALA	329	6.338	14.937	41.790	1.00	8.86
ATOM	2597	CB	ALA	329	5.774	13.738	42.559	1.00	8.82
ATOM	2598	C	ALA	329	6.251	16.142	42.687	1.00	9.58
ATOM	2599	O	ALA	329	7.205	16.498	43.351	1.00	10.57
ATOM	2600	N	PRO	330	5.072	16.776	42.730	1.00	9.98
ATOM	2601	CD	PRO	330	3.918	16.574	41.828	1.00	9.26
ATOM	2602	CA	PRO	330	4.870	17.948	43.589	1.00	10.35
ATOM	2603	CB	PRO	330	3.713	18.672	42.902	1.00	10.73
ATOM	2604	CG	PRO	330	2.866	17.515	42.414	1.00	9.12
ATOM	2605	C	PRO	330	4.438	17.374	44.944	1.00	12.06
ATOM	2606	O	PRO	330	4.293	16.164	45.091	1.00	10.37
ATOM	2607	N	PRO	331	4.230	18.235	45.951	1.00	13.60
ATOM	2608	CD	PRO	331	4.473	19.686	46.021	1.00	15.07
ATOM	2609	CA	PRO	331	3.800	17.705	47.245	1.00	14.74
ATOM	2610	CB	PRO	331	3.711	18.952	48.112	1.00	14.60
ATOM	2611	CG	PRO	331	4.720	19.890	47.500	1.00	16.16
ATOM	2612	C	PRO	331	2.429	17.094	47.021	1.00	14.60
ATOM	2613	O	PRO	331	1.735	17.506	46.088	1.00	14.09
ATOM	2614	N	GLN	332	2.006	16.167	47.882	1.00	15.86
ATOM	2615	CA	GLN	332	.700	15.541	47.679	1.00	16.96
ATOM	2616	CB	GLN	332	.530	14.272	48.520	1.00	18.42
ATOM	2617	CG	GLN	332	-.724	13.477	48.138	1.00	20.15
ATOM	2618	CD	GLN	332	-.663	12.036	48.596	1.00	20.82
ATOM	2619	OE1	GLN	332	.075	11.713	49.521	1.00	21.69
ATOM	2620	NE2	GLN	332	-1.446	11.165	47.957	1.00	21.22
ATOM	2621	C	GLN	332	-.464	16.476	47.923	1.00	17.13
ATOM	2622	O	GLN	332	-1.612	16.084	47.761	1.00	18.05
ATOM	2623	N	THR	333	-.169	17.714	48.304	1.00	17.02
ATOM	2624	CA	THR	333	-1.203	18.708	48.507	1.00	17.49
ATOM	2625	CB	THR	333	-.720	19.817	49.448	1.00	17.67
ATOM	2626	OG1	THR	333	.625	20.187	49.096	1.00	18.24
ATOM	2627	CG2	THR	333	-.778	19.331	50.908	1.00	18.95
ATOM	2628	C	THR	333	-1.591	19.342	47.167	1.00	16.95
ATOM	2629	O	THR	333	-2.406	20.272	47.125	1.00	17.72
ATOM	2630	N	TRP	334	-.983	18.846	46.084	1.00	15.03
ATOM	2631	CA	TRP	334	-1.246	19.333	44.727	1.00	15.17
ATOM	2632	CB	TRP	334	-.575	18.421	43.692	1.00	13.34
ATOM	2633	CG	TRP	334	-.727	18.886	42.250	1.00	12.07
ATOM	2634	CD2	TRP	334	-1.803	18.575	41.346	1.00	10.77
ATOM	2635	CE2	TRP	334	-1.536	19.244	40.129	1.00	10.12
ATOM	2636	CE3	TRP	334	-2.961	17.801	41.447	1.00	10.28
ATOM	2637	CD1	TRP	334	.123	19.709	41.556	1.00	11.34
ATOM	2638	NE1	TRP	334	-.357	19.926	40.280	1.00	10.68
ATOM	2639	CZ2	TRP	334	-2.393	19.157	39.021	1.00	9.02
ATOM	2640	CZ3	TRP	334	-3.817	17.714	40.345	1.00	10.49
ATOM	2641	CH2	TRP	334	-3.522	18.394	39.146	1.00	9.67
ATOM	2642	C	TRP	334	-2.752	19.349	44.493	1.00	15.09
ATOM	2643	O	TRP	334	-3.465	18.413	44.859	1.00	16.56
ATOM	2644	N	ASP	335	-3.231	20.393	43.832	1.00	15.99
ATOM	2645	CA	ASP	335	-4.654	20.543	43.603	1.00	17.37
ATOM	2646	CB	ASP	335	-5.239	21.164	44.870	1.00	20.66
ATOM	2647	CG	ASP	335	-6.735	21.089	44.936	1.00	23.84
ATOM	2648	OD1	ASP	335	-7.302	22.038	45.526	1.00	25.64
ATOM	2649	OD2	ASP	335	-7.343	20.101	44.425	1.00	25.81
ATOM	2650	C	ASP	335	-4.953	21.416	42.373	1.00	17.18
ATOM	2651	O	ASP	335	-5.633	22.442	42.470	1.00	18.93
ATOM	2652	N	GLY	336	-4.449	21.002	41.212	1.00	14.66
ATOM	2653	CA	GLY	336	-4.703	21.744	39.993	1.00	13.62

ATOM	2654	C	GLY	336	-3.467	22.363	39.381	1.00	12.61
ATOM	2655	O	GLY	336	-2.478	22.606	40.067	1.00	12.53
ATOM	2656	N	TYR	337	-3.529	22.606	38.076	1.00	11.81
ATOM	2657	CA	TYR	337	-2.421	23.208	37.351	1.00	11.63
ATOM	2658	CB	TYR	337	-2.349	22.654	35.929	1.00	9.96
ATOM	2659	CG	TYR	337	-2.006	21.200	35.871	1.00	8.29
ATOM	2660	CD1	TYR	337	-2.984	20.238	35.616	1.00	8.80
ATOM	2661	CE1	TYR	337	-2.649	18.884	35.547	1.00	7.99
ATOM	2662	CD2	TYR	337	-.695	20.779	36.061	1.00	8.21
ATOM	2663	CE2	TYR	337	-.353	19.452	35.996	1.00	8.96
ATOM	2664	CZ	TYR	337	-1.323	18.499	35.736	1.00	8.78
ATOM	2665	OH	TYR	337	-.940	17.175	35.648	1.00	9.08
ATOM	2666	C	TYR	337	-2.515	24.724	37.270	1.00	12.58
ATOM	2667	O	TYR	337	-3.607	25.292	37.202	1.00	14.26
ATOM	2668	N	ASP	338	-1.359	25.369	37.268	1.00	11.73
ATOM	2669	CA	ASP	338	-1.296	26.828	37.178	1.00	12.31
ATOM	2670	CB	ASP	338	-.389	27.361	38.294	1.00	13.40
ATOM	2671	CG	ASP	338	-.269	28.871	38.289	1.00	14.76
ATOM	2672	OD1	ASP	338	-.798	29.519	37.357	1.00	14.90
ATOM	2673	OD2	ASP	338	.370	29.392	39.232	1.00	17.31
ATOM	2674	C	ASP	338	-.714	27.166	35.799	1.00	11.47
ATOM	2675	O	ASP	338	.458	26.924	35.540	1.00	10.57
ATOM	2676	N	PRO	339	-1.535	27.727	34.895	1.00	11.07
ATOM	2677	CD	PRO	339	-2.902	28.241	35.092	1.00	13.23
ATOM	2678	CA	PRO	339	-1.039	28.066	33.554	1.00	11.38
ATOM	2679	CB	PRO	339	-2.289	28.586	32.847	1.00	12.85
ATOM	2680	CG	PRO	339	-3.036	29.253	33.962	1.00	14.27
ATOM	2681	C	PRO	339	.112	29.068	33.521	1.00	10.87
ATOM	2682	O	PRO	339	.783	29.213	32.499	1.00	11.32
ATOM	2683	N	SER	340	.340	29.773	34.628	1.00	10.79
ATOM	2684	CA	SER	340	1.434	30.739	34.664	1.00	10.82
ATOM	2685	CB	SER	340	1.276	31.719	35.820	1.00	12.00
ATOM	2686	OG	SER	340	1.545	31.088	37.058	1.00	14.09
ATOM	2687	C	SER	340	2.788	30.067	34.772	1.00	11.33
ATOM	2688	O	SER	340	3.821	30.739	34.731	1.00	12.52
ATOM	2689	N	TRP	341	2.794	28.744	34.947	1.00	10.94
ATOM	2690	CA	TRP	341	4.055	28.005	34.974	1.00	11.36
ATOM	2691	CB	TRP	341	3.898	26.626	35.616	1.00	11.69
ATOM	2692	CG	TRP	341	3.908	26.622	37.115	1.00	11.39
ATOM	2693	CD2	TRP	341	4.499	25.623	37.959	1.00	12.49
ATOM	2694	CE2	TRP	341	4.207	25.978	39.295	1.00	12.71
ATOM	2695	CE3	TRP	341	5.246	24.463	37.712	1.00	12.90
ATOM	2696	CD1	TRP	341	3.303	27.519	37.947	1.00	12.37
ATOM	2697	NE1	TRP	341	3.478	27.138	39.261	1.00	12.59
ATOM	2698	CZ2	TRP	341	4.639	25.209	40.386	1.00	13.77
ATOM	2699	CZ3	TRP	341	5.677	23.699	38.796	1.00	13.82
ATOM	2700	CH2	TRP	341	5.371	24.078	40.114	1.00	13.55
ATOM	2701	C	TRP	341	4.385	27.836	33.506	1.00	11.55
ATOM	2702	O	TRP	341	3.885	26.913	32.836	1.00	11.32
ATOM	2703	N	THR	342	5.225	28.741	33.013	1.00	11.51
ATOM	2704	CA	THR	342	5.608	28.751	31.614	1.00	12.18
ATOM	2705	CB	THR	342	5.332	30.141	30.986	1.00	12.46
ATOM	2706	OG1	THR	342	6.008	31.143	31.753	1.00	11.82
ATOM	2707	CG2	THR	342	3.842	30.441	30.997	1.00	12.94
ATOM	2708	C	THR	342	7.068	28.390	31.376	1.00	14.36
ATOM	2709	O	THR	342	7.464	28.230	30.208	1.00	14.94
ATOM	2710	OH2	TIP	100	-2.288	14.525	15.286	1.00	7.91
ATOM	2711	OH2	TIP	101	.343	8.794	35.546	1.00	8.49
ATOM	2712	OH2	TIP	102	-1.445	11.983	14.813	1.00	7.82
ATOM	2713	OH2	TIP	103	-1.755	-4.188	16.045	1.00	7.97

ATOM	2714	OH2	TIP	104	-2.996	18.702	27.914	1.00 8.56
ATOM	2715	OH2	TIP	105	3.203	35.557	17.130	1.00 11.80
ATOM	2716	OH2	TIP	106	-12.806	11.325	22.936	1.00 8.67
ATOM	2717	OH2	TIP	107	1.562	9.837	32.135	1.00 8.93
ATOM	2718	OH2	TIP	108	-3.239	-6.247	15.132	1.00 10.97
ATOM	2719	OH2	TIP	109	2.654	3.945	10.029	1.00 8.58
ATOM	2720	OH2	TIP	110	-5.295	22.040	30.655	1.00 11.77
ATOM	2721	OH2	TIP	111	2.831	9.995	36.021	1.00 9.91
ATOM	2722	OH2	TIP	112	-1.676	25.050	25.912	1.00 10.19
ATOM	2723	OH2	TIP	113	-2.489	24.433	13.659	1.00 11.40
ATOM	2724	OH2	TIP	114	3.967	.174	27.204	1.00 11.36
ATOM	2725	OH2	TIP	115	-.080	15.349	16.813	1.00 12.42
ATOM	2726	OH2	TIP	116	-9.271	.825	4.219	1.00 11.37
ATOM	2727	OH2	TIP	117	4.464	33.312	34.334	1.00 12.60
ATOM	2728	OH2	TIP	118	-5.905	23.511	4.817	1.00 11.48
ATOM	2729	OH2	TIP	119	1.200	35.846	19.081	1.00 12.50
ATOM	2730	OH2	TIP	120	-5.298	15.298	28.419	1.00 11.00
ATOM	2731	OH2	TIP	121	-1.625	-3.079	30.683	1.00 11.10
ATOM	2732	OH2	TIP	122	-14.668	9.646	27.217	1.00 11.16
ATOM	2733	OH2	TIP	123	-8.313	21.421	32.464	1.00 14.82
ATOM	2734	OH2	TIP	124	2.574	26.696	30.443	1.00 12.85
ATOM	2735	OH2	TIP	125	-1.911	21.086	28.882	1.00 11.28
ATOM	2736	OH2	TIP	126	-6.323	-4.344	36.182	1.00 15.61
ATOM	2737	OH2	TIP	127	-1.391	-13.992	23.661	1.00 12.14
ATOM	2738	OH2	TIP	128	.175	14.881	42.901	1.00 13.58
ATOM	2739	OH2	TIP	129	3.013	10.913	26.796	1.00 9.39
ATOM	2740	OH2	TIP	130	3.302	15.404	22.262	1.00 14.38
ATOM	2741	OH2	TIP	131	-4.137	24.008	32.627	1.00 12.80
ATOM	2742	OH2	TIP	132	2.071	-2.865	3.470	1.00 13.98
ATOM	2743	OH2	TIP	133	-13.641	21.431	25.146	1.00 13.70
ATOM	2744	OH2	TIP	134	6.846	6.168	31.408	1.00 13.28
ATOM	2745	OH2	TIP	135	.218	28.876	29.783	1.00 12.79
ATOM	2746	OH2	TIP	137	-4.794	-.568	40.350	1.00 13.73
ATOM	2747	OH2	TIP	138	-14.426	11.451	25.209	1.00 14.52
ATOM	2748	OH2	TIP	139	7.871	25.777	29.097	1.00 15.28
ATOM	2749	OH2	TIP	140	-6.443	4.909	-3.006	1.00 14.30
ATOM	2750	OH2	TIP	141	-19.445	14.193	15.780	1.00 15.63
ATOM	2751	OH2	TIP	142	20.494	4.563	31.333	1.00 16.44
ATOM	2752	OH2	TIP	143	-5.389	34.234	15.154	1.00 14.52
ATOM	2753	OH2	TIP	144	8.797	5.008	23.568	1.00 14.34
ATOM	2754	OH2	TIP	145	4.614	36.502	12.741	1.00 14.17
ATOM	2755	OH2	TIP	146	4.333	-11.138	21.353	1.00 14.65
ATOM	2756	OH2	TIP	147	9.270	7.368	30.201	1.00 13.66
ATOM	2757	OH2	TIP	148	-2.419	28.516	28.810	1.00 14.73
ATOM	2758	OH2	TIP	149	7.435	18.997	30.988	1.00 13.42
ATOM	2759	OH2	TIP	150	-15.793	18.325	6.391	1.00 15.97
ATOM	2760	OH2	TIP	151	.597	33.069	18.777	1.00 13.50
ATOM	2761	OH2	TIP	152	-8.182	-5.420	27.421	1.00 16.69
ATOM	2762	OH2	TIP	153	-6.019	22.024	36.715	1.00 14.75
ATOM	2763	OH2	TIP	154	5.534	3.296	36.812	1.00 15.77
ATOM	2764	OH2	TIP	155	-7.138	42.150	13.672	1.00 15.48
ATOM	2765	OH2	TIP	156	5.705	11.628	5.642	1.00 15.17
ATOM	2766	OH2	TIP	157	10.027	-5.088	24.931	1.00 16.42
ATOM	2767	OH2	TIP	158	-7.378	27.977	9.820	1.00 15.87
ATOM	2768	OH2	TIP	159	4.176	10.191	33.639	1.00 15.02
ATOM	2769	OH2	TIP	160	-9.151	28.753	24.512	1.00 16.13
ATOM	2770	OH2	TIP	161	-.280	22.847	14.207	1.00 20.47
ATOM	2771	OH2	TIP	162	-5.754	21.957	33.742	1.00 16.70
ATOM	2772	OH2	TIP	163	-1.842	22.693	42.796	1.00 16.49
ATOM	2773	OH2	TIP	164	2.945	38.943	12.063	1.00 15.34

ATOM	2774	OH2	TIP	165	10.286	9.083	17.158	1.00 17.27
ATOM	2775	OH2	TIP	166	-8.657	-10.867	22.407	1.00 15.36
ATOM	2776	OH2	TIP	167	-4.144	1.834	38.912	1.00 14.58
ATOM	2777	OH2	TIP	168	7.159	10.030	30.911	1.00 13.59
ATOM	2778	OH2	TIP	169	1.090	23.926	37.021	1.00 18.03
ATOM	2779	OH2	TIP	170	5.020	1.037	-1.123	1.00 17.94
ATOM	2780	OH2	TIP	171	8.222	15.533	31.128	1.00 13.48
ATOM	2781	OH2	TIP	172	1.010	-7.143	14.214	1.00 14.38
ATOM	2782	OH2	TIP	173	-2.383	29.347	25.884	1.00 14.99
ATOM	2783	OH2	TIP	174	-11.374	3.360	3.691	1.00 19.15
ATOM	2784	OH2	TIP	175	6.650	7.626	-2.161	1.00 16.21
ATOM	2785	OH2	TIP	176	-1.619	-7.372	13.203	1.00 18.99
ATOM	2786	OH2	TIP	177	-5.374	25.402	34.790	1.00 20.42
ATOM	2787	OH2	TIP	178	-3.590	-8.334	33.021	1.00 18.30
ATOM	2788	OH2	TIP	179	3.880	21.790	-1.507	1.00 21.02
ATOM	2789	OH2	TIP	180	17.269	3.354	32.211	1.00 18.66
ATOM	2790	OH2	TIP	181	-9.324	26.271	11.523	1.00 17.31
ATOM	2791	OH2	TIP	182	19.465	6.850	39.697	1.00 16.33
ATOM	2792	OH2	TIP	183	-12.325	23.377	4.184	1.00 13.09
ATOM	2793	OH2	TIP	184	-.590	1.220	45.203	1.00 22.04
ATOM	2794	OH2	TIP	185	.238	3.021	35.566	1.00 16.78
ATOM	2795	OH2	TIP	186	13.358	15.194	46.398	1.00 14.89
ATOM	2796	OH2	TIP	187	9.068	-.545	35.512	1.00 16.41
ATOM	2797	OH2	TIP	188	18.659	6.840	32.004	1.00 21.41
ATOM	2798	OH2	TIP	189	-2.204	21.394	5.836	1.00 22.27
ATOM	2799	OH2	TIP	190	6.399	-7.859	31.845	1.00 15.37
ATOM	2800	OH2	TIP	191	6.568	-8.956	18.513	1.00 18.80
ATOM	2801	OH2	TIP	192	-8.990	31.008	16.862	1.00 20.51
ATOM	2802	OH2	TIP	193	14.719	-1.322	29.679	1.00 19.14
ATOM	2803	OH2	TIP	194	-4.307	-4.427	5.440	1.00 22.95
ATOM	2804	OH2	TIP	195	3.370	32.428	6.730	1.00 18.69
ATOM	2805	OH2	TIP	196	2.044	13.568	2.631	1.00 18.66
ATOM	2806	OH2	TIP	197	-10.401	6.446	-2.842	1.00 20.08
ATOM	2807	OH2	TIP	198	9.626	-6.433	34.738	1.00 25.30
ATOM	2808	OH2	TIP	199	8.514	6.421	1.801	1.00 21.78
ATOM	2809	OH2	TIP	200	-17.207	9.678	27.696	1.00 21.94
ATOM	2810	OH2	TIP	201	2.919	4.179	-6.333	1.00 18.70
ATOM	2811	OH2	TIP	202	6.361	28.436	41.243	1.00 19.89
ATOM	2812	OH2	TIP	203	-10.262	-3.957	26.833	1.00 19.46
ATOM	2813	OH2	TIP	204	9.331	5.080	31.737	1.00 18.15
ATOM	2814	OH2	TIP	205	6.857	-.672	12.552	1.00 19.07
ATOM	2815	OH2	TIP	206	-2.168	14.371	44.153	1.00 20.04
ATOM	2816	OH2	TIP	207	15.929	6.453	22.090	1.00 18.88
ATOM	2817	OH2	TIP	208	3.843	15.020	49.813	1.00 19.72
ATOM	2818	OH2	TIP	209	-5.404	-4.250	3.054	1.00 21.83
ATOM	2819	OH2	TIP	210	-1.315	32.050	22.928	1.00 23.31
ATOM	2820	OH2	TIP	211	-4.204	7.216	47.364	1.00 20.27
ATOM	2821	OH2	TIP	212	18.020	6.772	25.404	1.00 22.66
ATOM	2822	OH2	TIP	213	.307	-13.876	25.899	1.00 16.03
ATOM	2823	OH2	TIP	214	-6.377	-2.487	39.729	1.00 22.66
ATOM	2824	OH2	TIP	215	21.003	13.410	33.591	1.00 21.35
ATOM	2825	OH2	TIP	216	-3.503	-8.251	27.038	1.00 24.52
ATOM	2826	OH2	TIP	217	-9.805	7.228	43.867	1.00 18.58
ATOM	2827	OH2	TIP	218	-12.846	-2.117	20.687	1.00 19.69
ATOM	2828	OH2	TIP	219	-7.448	8.660	-5.433	1.00 20.76
ATOM	2829	OH2	TIP	220	4.026	-9.653	24.723	1.00 19.35
ATOM	2830	OH2	TIP	221	1.351	43.326	13.087	1.00 21.08
ATOM	2831	OH2	TIP	222	7.202	-7.998	34.393	1.00 22.08
ATOM	2832	OH2	TIP	223	-2.390	19.119	7.073	1.00 22.59
ATOM	2833	OH2	TIP	224	-21.821	8.242	16.465	1.00 27.25

ATOM	2834	OH2	TIP	225	-6.782	13.407	38.563	1.00 22.55
ATOM	2835	OH2	TIP	226	-10.549	3.747	-2.525	1.00 17.81
ATOM	2836	OH2	TIP	227	-8.036	11.901	35.618	1.00 17.69
ATOM	2837	OH2	TIP	228	-12.553	13.986	-1.899	1.00 22.63
ATOM	2838	OH2	TIP	229	19.507	2.749	39.442	1.00 20.77
ATOM	2839	OH2	TIP	230	2.467	12.552	50.689	1.00 24.86
ATOM	2840	OH2	TIP	231	7.195	9.071	-4.482	1.00 22.53
ATOM	2841	OH2	TIP	232	9.515	-2.944	23.235	1.00 24.15
ATOM	2842	OH2	TIP	233	5.532	-8.311	28.811	1.00 18.76
ATOM	2843	OH2	TIP	234	7.942	-8.611	27.938	1.00 20.44
ATOM	2844	OH2	TIP	235	-20.541	9.765	14.299	1.00 19.63
ATOM	2845	OH2	TIP	236	8.817	3.612	1.850	1.00 22.41
ATOM	2846	OH2	TIP	237	-7.787	-6.751	18.579	1.00 19.42
ATOM	2847	OH2	TIP	238	-.436	19.416	13.690	1.00 22.78
ATOM	2848	OH2	TIP	239	15.797	17.444	45.082	1.00 28.40
ATOM	2849	OH2	TIP	240	1.925	13.354	27.630	1.00 18.62
ATOM	2850	OH2	TIP	241	-5.215	17.779	-2.017	1.00 20.16
ATOM	2851	OH2	TIP	242	12.890	13.271	20.583	1.00 22.91
ATOM	2852	OH2	TIP	243	-14.719	17.252	32.242	1.00 22.96
ATOM	2853	OH2	TIP	244	12.026	1.784	46.150	1.00 22.48
ATOM	2854	OH2	TIP	245	-11.786	.621	3.517	1.00 23.43
ATOM	2855	OH2	TIP	246	-9.210	33.679	5.141	1.00 24.67
ATOM	2856	OH2	TIP	247	14.956	26.443	37.050	1.00 21.23
ATOM	2857	OH2	TIP	248	1.994	19.240	-7.436	1.00 23.93
ATOM	2858	OH2	TIP	249	4.719	11.134	50.914	1.00 26.21
ATOM	2859	OH2	TIP	250	-9.759	-2.036	2.345	1.00 29.03
ATOM	2860	OH2	TIP	251	22.302	2.304	51.200	1.00 22.37
ATOM	2861	OH2	TIP	252	.754	17.381	18.903	1.00 28.71
ATOM	2862	OH2	TIP	253	10.842	-3.173	21.160	1.00 20.86
ATOM	2863	OH2	TIP	254	16.509	25.320	35.043	1.00 28.06
ATOM	2864	OH2	TIP	255	1.209	-9.441	30.784	1.00 23.18
ATOM	2865	OH2	TIP	256	-14.814	14.622	32.926	1.00 23.24
ATOM	2866	OH2	TIP	257	10.945	26.110	43.061	1.00 22.48
ATOM	2867	OH2	TIP	258	23.167	4.355	52.538	1.00 25.76
ATOM	2868	OH2	TIP	259	-8.639	-10.256	35.742	1.00 25.25
ATOM	2869	OH2	TIP	260	-4.932	29.011	19.115	1.00 25.86
ATOM	2870	OH2	TIP	261	2.414	20.831	38.688	1.00 29.42
ATOM	2871	OH2	TIP	262	-3.125	-1.778	-2.464	1.00 20.61
ATOM	2872	OH2	TIP	263	19.240	21.513	35.973	1.00 22.61
ATOM	2873	OH2	TIP	264	24.254	2.439	45.656	1.00 29.38
ATOM	2874	OH2	TIP	265	10.937	9.304	52.114	1.00 26.11
ATOM	2875	OH2	TIP	266	-1.318	6.351	-8.990	1.00 25.46
ATOM	2876	OH2	TIP	267	8.531	31.698	32.310	1.00 28.78
ATOM	2877	OH2	TIP	268	-18.198	17.905	7.340	1.00 25.41
ATOM	2878	OH2	TIP	269	-6.273	29.517	27.892	1.00 25.61
ATOM	2879	OH2	TIP	270	-11.732	28.604	20.442	1.00 24.07
ATOM	2880	OH2	TIP	271	7.692	1.763	2.975	1.00 28.01
ATOM	2881	OH2	TIP	272	-5.478	16.120	37.074	1.00 27.80
ATOM	2882	OH2	TIP	273	11.578	7.355	5.644	1.00 26.68
ATOM	2883	OH2	TIP	274	-9.219	30.120	19.649	1.00 22.55
ATOM	2884	OH2	TIP	275	-16.959	.619	27.213	1.00 22.05
ATOM	2885	OH2	TIP	276	-4.504	24.109	1.731	1.00 21.57
ATOM	2886	OH2	TIP	277	-5.775	32.281	-2.195	1.00 23.97
ATOM	2887	OH2	TIP	278	-15.964	-1.806	8.142	1.00 31.06
ATOM	2888	OH2	TIP	279	-18.453	23.170	22.854	1.00 22.03
ATOM	2889	OH2	TIP	280	-20.496	16.171	23.020	1.00 26.44
ATOM	2890	OH2	TIP	281	24.522	11.231	36.110	1.00 27.02
ATOM	2891	OH2	TIP	282	-9.974	22.866	34.203	1.00 25.77
ATOM	2892	OH2	TIP	283	16.946	-2.262	43.083	1.00 27.85
ATOM	2893	OH2	TIP	284	8.204	17.950	-7.140	1.00 24.42

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ATOM   2894  OH2 TIP   287      21.968   1.318  37.353  1.00 27.82
ATOM   2895  OH2 TIP   288     -12.016    .453    .495  1.00 23.18
ATOM   2896  OH2 TIP   289       9.134   7.198   -.859  1.00 19.54
ATOM   2897  OH2 TIP   290     -21.242  12.609  14.359  1.00 25.05
ATOM   2898  OH2 TIP   291      -6.351  29.809  31.947  1.00 26.79
ATOM   2899  OH2 TIP   292       1.180  31.885  40.083  1.00 26.06
ATOM   2900  OH2 TIP   293     -16.325   1.287   7.220  1.00 24.22
ATOM   2901  OH2 TIP   294      18.186   1.597  52.152  1.00 23.20
ATOM   2902  OH2 TIP   295     -12.173  24.331  32.021  1.00 28.41
ATOM   2903  OH2 TIP   296     -19.262   1.630  13.392  1.00 31.63
ATOM   2904  OH2 TIP   297       5.507   2.842  46.560  1.00 21.56
ATOM   2905  OH2 TIP   298     -12.466   2.686   -.729  1.00 32.83
ATOM   2906  OH2 TIP   299      -2.368   8.417  48.553  1.00 23.93
ATOM   2907  OH2 TIP   300       9.657   2.419   -.625  1.00 26.98
ATOM   2908  OH2 TIP   301      17.591   1.180  41.208  1.00 29.88
ATOM   2909  OH2 TIP   302      15.260  18.610  29.612  1.00 30.53
ATOM   2910  OH2 TIP   303      -8.663  -2.353  38.760  1.00 27.60
ATOM   2911  OH2 TIP   304      13.764  -6.406  28.754  1.00 31.17
ATOM   2912  OH2 TIP   305     -15.114   8.860   -.237  1.00 27.49
ATOM   2913  OH2 TIP   306      18.214  12.233  49.633  1.00 24.66
ATOM   2914  OH2 TIP   307     -18.413  -1.792  15.629  1.00 26.42
ATOM   2915  OH2 TIP   308      -7.173  14.274  34.805  1.00 22.11
ATOM   2916  OH2 TIP   309      -8.205   6.238  -4.579  1.00 23.83
ATOM   2917  OH2 TIP   310      13.895   9.443   9.960  1.00 27.01
ATOM   2918  OH2 TIP   311      -8.520  32.700   9.680  1.00 29.23
ATOM   2919  OH2 TIP   312     -21.376  20.151  17.437  1.00 22.96
ATOM   2920  OH2 TIP   313     -18.193   1.488  18.353  1.00 26.17
ATOM   2921  OH2 TIP   314     -12.319  26.640   4.016  1.00 23.06
ATOM   2922  OH2 TIP   315      -7.632  36.261  10.439  1.00 27.49
ATOM   2923  OH2 TIP   316     -18.891   7.671  25.883  1.00 24.79
ATOM   2924  OH2 TIP   317       2.956   6.449  -7.864  1.00 27.90
ATOM   2925  OH2 TIP   318      14.563    .423  26.984  1.00 23.53
ATOM   2926  OH2 TIP   319     -16.552  13.238  25.846  1.00 32.62
ATOM   2927  OH2 TIP   320      23.897  13.508  34.577  1.00 30.60
ATOM   2928  OH2 TIP   321      -6.850 -10.660  31.700  1.00 28.92
ATOM   2929  OH2 TIP   323       2.865  24.012  17.343  1.00 40.19
ATOM   2930  OH2 TIP   324      -6.445  28.095  34.181  1.00 25.33
ATOM   2931  OH2 TIP   326     -12.804  -8.543  10.804  1.00 27.30
ATOM   2932  OH2 TIP   327     -15.923  20.258   9.884  1.00 25.55
ATOM   2933  OH2 TIP   328      19.921  17.422  45.448  1.00 27.92
ATOM   2934  OH2 TIP   329     -10.255  29.085   5.082  1.00 27.81
ATOM   2935  OH2 TIP   330     -17.685    .819  15.657  1.00 29.54
ATOM   2936  OH2 TIP   331      13.918  -1.760  45.050  1.00 30.37
ATOM   2937  OH2 TIP   332       1.126  -8.513   9.655  1.00 31.74
ATOM   2938  OH2 TIP   334     -12.495  27.938  24.336  1.00 26.25
ATOM   2939  OH2 TIP   335       7.775  30.223  34.373  1.00 26.90
ATOM   2940  OH2 TIP   336       5.389  21.840  43.001  1.00 28.62
ATOM   2941  OH2 TIP   338       6.067  24.754  25.830  1.00 28.09
ATOM   2942  OH2 TIP   339      -8.753  17.532  40.860  1.00 36.42
ATOM   2943  OH2 TIP   340      12.557   2.947  17.296  1.00 24.95
ATOM   2944  OH2 TIP   341      12.877  12.867  27.503  1.00 24.86
ATOM   2945  OH2 TIP   342     -12.082  21.787  45.600  1.00 28.19
ATOM   2946  OH2 TIP   343      16.107   4.184  20.081  1.00 32.31
ATOM   2947  OH2 TIP   344      -7.072  19.107  -2.845  1.00 30.93
END
```

Table 2

```
REMARK GnT-1 structure with MeHg bound, "gnt1f"
REMARK Ulug Unligil, 1999 06 11
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.5 A
REMARK starting r=  .2545 free_r=  .2672
REMARK final    r=  .2369 free_r=  .2501
REMARK B rmsd for bonded mainchain atoms=   .840  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  1.595  target= 2.0
REMARK B rmsd for angle mainchain atoms=  1.299  target= 2.0
REMARK B rmsd for angle sidechain atoms=  2.451  target= 2.5
REMARK wa= .901697
REMARK rweight=.157734
REMARK target= mlf  steps= 30
REMARK sg= P2(1)2(1)2(1) a= 40.382 b= 82.378 c= 102.487 alpha= 90 beta=
90 gamma= 90
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : ../data/mmc.param
REMARK parameter file 3  : CNS_TOPPAR:water_rep.param
REMARK molecular structure file: generate_easy.mtf
REMARK input coordinates: bgroup.ann.pdb
REMARK reflection file= ../data/gnt1_start.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.5
REMARK initial B-factor correction applied to f_wl :
REMARK   B11=   -.069 B22=   1.877 B33=  -1.809
REMARK   B12=    .000 B13=    .000 B23=    .000
REMARK B-factor correction applied to coordinate array B:    -.760
REMARK bulk solvent: density level= .377577 e/A^3, B-factor= 29.956 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range:    105746 (
100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  22053 (
20.9 % )
REMARK number of reflections rejected:                            0 (
.0 % )
REMARK total number of reflections used:                      83693 (
79.1 % )
REMARK number of reflections in working set:                  79589 (
75.3 % )
REMARK number of reflections in test set:                      4104 (
3.9 % )
REMARK FILENAME="bindividual.ann.pdb"
REMARK DATE:11-Jun-99  11:49:39       created by user: ulu
REMARK VERSION:0.5
ATOM      1  CB  ALA     1     -15.508  -1.587  18.267  1.00 17.32
ATOM      2  C   ALA     1     -14.658  -2.056  15.988  1.00 17.45
ATOM      3  O   ALA     1     -13.441  -2.192  15.872  1.00 18.11
ATOM      4  N   ALA     1     -14.630  -3.810  17.724  1.00 16.06
ATOM      5  CA  ALA     1     -15.379  -2.639  17.188  1.00 16.83
ATOM      6  N   VAL     2     -15.410  -1.407  15.097  1.00 16.97
ATOM      7  CA  VAL     2     -14.820   -.774  13.914  1.00 16.50
ATOM      8  CB  VAL     2     -15.872   -.587  12.784  1.00 16.65
ATOM      9  CG1 VAL     2     -15.292    .279  11.656  1.00 16.57
ATOM     10  CG2 VAL     2     -16.278  -1.945  12.238  1.00 17.55
ATOM     11  C   VAL     2     -14.252    .589  14.331  1.00 15.10
ATOM     12  O   VAL     2     -14.944   1.394  14.954  1.00 15.19
```

ATOM	13	N	ILE	3	-12.979	.826	14.018	1.00	13.05
ATOM	14	CA	ILE	3	-12.303	2.074	14.356	1.00	12.08
ATOM	15	CB	ILE	3	-11.308	1.879	15.522	1.00	12.25
ATOM	16	CG2	ILE	3	-10.683	3.239	15.879	1.00	11.93
ATOM	17	CG1	ILE	3	-12.024	1.268	16.741	1.00	12.56
ATOM	18	CD1	ILE	3	-11.096	.835	17.865	1.00	12.66
ATOM	19	C	ILE	3	-11.517	2.540	13.130	1.00	11.41
ATOM	20	O	ILE	3	-10.537	1.902	12.729	1.00	11.23
ATOM	21	N	PRO	4	-11.930	3.657	12.518	1.00	9.62
ATOM	22	CD	PRO	4	-13.067	4.563	12.778	1.00	10.29
ATOM	23	CA	PRO	4	-11.171	4.084	11.344	1.00	8.48
ATOM	24	CB	PRO	4	-12.144	5.033	10.643	1.00	9.98
ATOM	25	CG	PRO	4	-12.820	5.713	11.804	1.00	9.23
ATOM	26	C	PRO	4	-9.857	4.763	11.711	1.00	8.53
ATOM	27	O	PRO	4	-9.702	5.314	12.815	1.00	7.56
ATOM	28	N	ILE	5	-8.906	4.690	10.793	1.00	8.42
ATOM	29	CA	ILE	5	-7.633	5.357	10.982	1.00	8.19
ATOM	30	CB	ILE	5	-6.432	4.439	10.642	1.00	9.81
ATOM	31	CG2	ILE	5	-5.112	5.169	10.936	1.00	9.44
ATOM	32	CG1	ILE	5	-6.525	3.123	11.438	1.00	9.99
ATOM	33	CD1	ILE	5	-6.543	3.273	12.946	1.00	10.77
ATOM	34	C	ILE	5	-7.694	6.526	9.998	1.00	8.61
ATOM	35	O	ILE	5	-7.901	6.325	8.799	1.00	8.89
ATOM	36	N	LEU	6	-7.535	7.742	10.505	1.00	7.16
ATOM	37	CA	LEU	6	-7.573	8.924	9.656	1.00	7.79
ATOM	38	CB	LEU	6	-8.407	10.023	10.311	1.00	8.49
ATOM	39	CG	LEU	6	-8.402	11.398	9.622	1.00	8.93
ATOM	40	CD1	LEU	6	-9.014	11.297	8.215	1.00	10.56
ATOM	41	CD2	LEU	6	-9.179	12.397	10.472	1.00	10.91
ATOM	42	C	LEU	6	-6.141	9.397	9.495	1.00	7.08
ATOM	43	O	LEU	6	-5.518	9.816	10.460	1.00	7.28
ATOM	44	N	VAL	7	-5.627	9.319	8.277	1.00	6.74
ATOM	45	CA	VAL	7	-4.260	9.742	7.991	1.00	6.91
ATOM	46	CB	VAL	7	-3.617	8.799	6.945	1.00	5.89
ATOM	47	CG1	VAL	7	-2.219	9.256	6.592	1.00	7.60
ATOM	48	CG2	VAL	7	-3.607	7.375	7.464	1.00	5.76
ATOM	49	C	VAL	7	-4.264	11.171	7.432	1.00	7.45
ATOM	50	O	VAL	7	-4.918	11.435	6.426	1.00	7.22
ATOM	51	N	ILE	8	-3.534	12.080	8.079	1.00	7.61
ATOM	52	CA	ILE	8	-3.459	13.466	7.636	1.00	9.24
ATOM	53	CB	ILE	8	-3.332	14.455	8.815	1.00	10.41
ATOM	54	CG2	ILE	8	-3.114	15.869	8.270	1.00	10.46
ATOM	55	CG1	ILE	8	-4.608	14.441	9.669	1.00	12.20
ATOM	56	CD1	ILE	8	-4.846	13.185	10.442	1.00	16.13
ATOM	57	C	ILE	8	-2.243	13.616	6.739	1.00	9.52
ATOM	58	O	ILE	8	-1.107	13.470	7.182	1.00	10.12
ATOM	59	N	ALA	9	-2.484	13.932	5.476	1.00	8.88
ATOM	60	CA	ALA	9	-1.407	14.053	4.509	1.00	10.10
ATOM	61	CB	ALA	9	-1.425	12.848	3.574	1.00	9.54
ATOM	62	C	ALA	9	-1.470	15.326	3.698	1.00	10.42
ATOM	63	O	ALA	9	-2.495	16.006	3.669	1.00	10.45
ATOM	64	N	CYS	10	-.367	15.636	3.021	1.00	13.39
ATOM	65	CA	CYS	10	-.325	16.854	2.224	1.00	15.20
ATOM	66	C	CYS	10	.674	16.836	1.074	1.00	15.60
ATOM	67	O	CYS	10	.282	16.575	-.065	1.00	16.64
ATOM	68	CB	CYS	10	-.103	18.059	3.162	1.00	17.60
ATOM	69	SG	CYS	10	.587	19.619	2.506	1.00	20.39
ATOM	70	N	ASP	11	1.950	17.101	1.352	1.00	16.86
ATOM	71	CA	ASP	11	2.946	17.153	.279	1.00	17.00
ATOM	72	CB	ASP	11	3.234	18.624	-.049	1.00	18.36

ATOM	73	CG	ASP	11	3.647	19.431	1.175	1.00	18.09
ATOM	74	OD1	ASP	11	3.821	20.667	1.053	1.00	18.37
ATOM	75	OD2	ASP	11	3.811	18.839	2.267	1.00	18.53
ATOM	76	C	ASP	11	4.251	16.394	.519	1.00	18.58
ATOM	77	O	ASP	11	5.337	16.870	.157	1.00	18.26
ATOM	78	N	ARG	12	4.148	15.228	1.154	1.00	18.01
ATOM	79	CA	ARG	12	5.306	14.380	1.413	1.00	17.77
ATOM	80	CB	ARG	12	5.596	14.296	2.916	1.00	20.91
ATOM	81	CG	ARG	12	6.055	15.603	3.546	1.00	23.63
ATOM	82	CD	ARG	12	6.360	15.410	5.049	1.00	26.88
ATOM	83	NE	ARG	12	7.728	15.799	5.415	1.00	30.67
ATOM	84	CZ	ARG	12	8.226	17.032	5.302	1.00	32.26
ATOM	85	NH1	ARG	12	7.474	18.025	4.825	1.00	33.50
ATOM	86	NH2	ARG	12	9.474	17.280	5.681	1.00	33.19
ATOM	87	C	ARG	12	5.007	12.991	.846	1.00	17.04
ATOM	88	O	ARG	12	4.137	12.262	1.345	1.00	15.66
ATOM	89	N	SER	13	5.740	12.624	-.196	1.00	16.52
ATOM	90	CA	SER	13	5.551	11.336	-.836	1.00	15.99
ATOM	91	CB	SER	13	6.454	11.217	-2.063	1.00	16.72
ATOM	92	OG	SER	13	7.809	11.098	-1.686	1.00	16.77
ATOM	93	C	SER	13	5.826	10.189	.123	1.00	15.73
ATOM	94	O	SER	13	5.380	9.063	-.112	1.00	14.86
ATOM	95	N	THR	14	6.562	10.476	1.197	1.00	14.85
ATOM	96	CA	THR	14	6.878	9.468	2.198	1.00	14.82
ATOM	97	CB	THR	14	8.005	9.967	3.155	1.00	15.41
ATOM	98	OG1	THR	14	7.631	11.214	3.752	1.00	16.90
ATOM	99	CG2	THR	14	9.308	10.167	2.375	1.00	16.09
ATOM	100	C	THR	14	5.630	9.015	3.001	1.00	14.09
ATOM	101	O	THR	14	5.736	8.255	3.961	1.00	13.39
ATOM	102	N	VAL	15	4.443	9.476	2.606	1.00	12.61
ATOM	103	CA	VAL	15	3.229	9.010	3.273	1.00	12.42
ATOM	104	CB	VAL	15	1.937	9.748	2.761	1.00	11.57
ATOM	105	CG1	VAL	15	1.819	9.648	1.248	1.00	13.45
ATOM	106	CG2	VAL	15	.690	9.157	3.415	1.00	12.72
ATOM	107	C	VAL	15	3.178	7.512	2.936	1.00	11.40
ATOM	108	O	VAL	15	2.466	6.734	3.560	1.00	11.88
ATOM	109	N	ARG	16	3.976	7.116	1.943	1.00	11.41
ATOM	110	CA	ARG	16	4.065	5.721	1.517	1.00	10.83
ATOM	111	CB	ARG	16	5.050	5.593	.347	1.00	10.67
ATOM	112	CG	ARG	16	5.329	4.145	-.087	1.00	10.78
ATOM	113	CD	ARG	16	6.423	4.080	-1.158	1.00	12.75
ATOM	114	NE	ARG	16	6.051	4.745	-2.403	1.00	12.35
ATOM	115	CZ	ARG	16	5.246	4.226	-3.328	1.00	12.75
ATOM	116	NH1	ARG	16	4.721	3.025	-3.151	1.00	13.12
ATOM	117	NH2	ARG	16	4.971	4.907	-4.438	1.00	13.25
ATOM	118	C	ARG	16	4.529	4.837	2.674	1.00	10.88
ATOM	119	O	ARG	16	3.990	3.748	2.884	1.00	10.44
ATOM	120	N	ARG	17	5.535	5.293	3.417	1.00	11.34
ATOM	121	CA	ARG	17	6.062	4.527	4.545	1.00	11.75
ATOM	122	CB	ARG	17	7.319	5.204	5.109	1.00	13.29
ATOM	123	CG	ARG	17	7.872	4.564	6.395	1.00	15.73
ATOM	124	CD	ARG	17	9.224	5.171	6.775	1.00	18.58
ATOM	125	NE	ARG	17	9.698	4.787	8.111	1.00	20.92
ATOM	126	CZ	ARG	17	10.847	5.223	8.628	1.00	21.77
ATOM	127	NH1	ARG	17	11.607	6.035	7.914	1.00	22.36
ATOM	128	NH2	ARG	17	11.243	4.861	9.849	1.00	23.18
ATOM	129	C	ARG	17	5.021	4.396	5.633	1.00	11.62
ATOM	130	O	ARG	17	4.888	3.342	6.258	1.00	10.96
ATOM	131	N	CYS	18	4.293	5.485	5.858	1.00	10.37
ATOM	132	CA	CYS	18	3.238	5.521	6.860	1.00	10.30

ATOM	133	CB	CYS	18	2.672	6.951	6.955	1.00	10.22
ATOM	134	SG	CYS	18	.919	7.110	7.478	1.00	11.83
ATOM	135	C	CYS	18	2.137	4.524	6.484	1.00	9.67
ATOM	136	O	CYS	18	1.701	3.722	7.312	1.00	8.70
ATOM	137	N	LEU	19	1.727	4.545	5.220	1.00	9.23
ATOM	138	CA	LEU	19	.677	3.655	4.764	1.00	9.64
ATOM	139	CB	LEU	19	.151	4.089	3.391	1.00	9.70
ATOM	140	CG	LEU	19	-.610	5.424	3.355	1.00	11.63
ATOM	141	CD1	LEU	19	-1.151	5.727	1.937	1.00	10.99
ATOM	142	CD2	LEU	19	-1.735	5.343	4.353	1.00	10.89
ATOM	143	C	LEU	19	1.138	2.200	4.713	1.00	9.44
ATOM	144	O	LEU	19	.387	1.294	5.073	1.00	9.45
ATOM	145	N	ASP	20	2.374	1.962	4.289	1.00	9.93
ATOM	146	CA	ASP	20	2.840	.581	4.209	1.00	10.03
ATOM	147	CB	ASP	20	4.242	.506	3.602	1.00	10.95
ATOM	148	CG	ASP	20	4.254	.819	2.113	1.00	12.40
ATOM	149	OD1	ASP	20	3.180	.787	1.462	1.00	13.20
ATOM	150	OD2	ASP	20	5.357	1.076	1.587	1.00	13.24
ATOM	151	C	ASP	20	2.838	-.098	5.569	1.00	10.42
ATOM	152	O	ASP	20	2.466	-1.266	5.684	1.00	10.06
ATOM	153	N	LYS	21	3.257	.631	6.597	1.00	10.96
ATOM	154	CA	LYS	21	3.284	.068	7.938	1.00	11.53
ATOM	155	CB	LYS	21	4.075	.985	8.869	1.00	13.63
ATOM	156	CG	LYS	21	5.570	.924	8.647	1.00	16.64
ATOM	157	CD	LYS	21	6.119	-.411	9.101	1.00	18.26
ATOM	158	CE	LYS	21	7.627	-.481	8.890	1.00	21.15
ATOM	159	NZ	LYS	21	7.977	-.115	7.507	1.00	23.16
ATOM	160	C	LYS	21	1.872	-.158	8.472	1.00	11.34
ATOM	161	O	LYS	21	1.589	-1.190	9.082	1.00	11.27
ATOM	162	N	LEU	22	.983	.808	8.251	1.00	10.98
ATOM	163	CA	LEU	22	-.392	.664	8.707	1.00	9.91
ATOM	164	CB	LEU	22	-1.203	1.903	8.368	1.00	8.45
ATOM	165	CG	LEU	22	-1.032	3.125	9.263	1.00	7.20
ATOM	166	CD1	LEU	22	-1.639	4.323	8.544	1.00	7.53
ATOM	167	CD2	LEU	22	-1.727	2.897	10.606	1.00	8.28
ATOM	168	C	LEU	22	-1.037	-.548	8.040	1.00	10.04
ATOM	169	O	LEU	22	-1.666	-1.363	8.705	1.00	9.59
ATOM	170	N	LEU	23	-.851	-.672	6.727	1.00	9.01
ATOM	171	CA	LEU	23	-1.421	-1.786	5.978	1.00	9.26
ATOM	172	CB	LEU	23	-1.305	-1.506	4.474	1.00	10.13
ATOM	173	CG	LEU	23	-2.257	-.398	3.991	1.00	10.33
ATOM	174	CD1	LEU	23	-1.945	.007	2.552	1.00	11.51
ATOM	175	CD2	LEU	23	-3.673	-.898	4.096	1.00	10.83
ATOM	176	C	LEU	23	-.802	-3.144	6.329	1.00	9.26
ATOM	177	O	LEU	23	-1.491	-4.168	6.347	1.00	9.95
ATOM	178	N	HIS	24	.492	-3.152	6.617	1.00	9.05
ATOM	179	CA	HIS	24	1.177	-4.386	6.978	1.00	9.34
ATOM	180	CB	HIS	24	2.685	-4.165	7.058	1.00	10.21
ATOM	181	CG	HIS	24	3.431	-5.375	7.519	1.00	11.78
ATOM	182	CD2	HIS	24	3.921	-5.710	8.735	1.00	12.38
ATOM	183	ND1	HIS	24	3.641	-6.469	6.706	1.00	14.09
ATOM	184	CE1	HIS	24	4.225	-7.427	7.403	1.00	12.66
ATOM	185	NE2	HIS	24	4.405	-6.992	8.638	1.00	14.41
ATOM	186	C	HIS	24	.707	-4.953	8.321	1.00	10.14
ATOM	187	O	HIS	24	.550	-6.166	8.481	1.00	10.54
ATOM	188	N	TYR	25	.505	-4.076	9.293	1.00	9.32
ATOM	189	CA	TYR	25	.074	-4.521	10.607	1.00	9.71
ATOM	190	CB	TYR	25	.740	-3.660	11.685	1.00	9.07
ATOM	191	CG	TYR	25	2.217	-3.953	11.833	1.00	9.57
ATOM	192	CD1	TYR	25	3.158	-2.947	11.737	1.00	11.61

ATOM	193	CE1	TYR	25	4.524	-3.219	11.896	1.00	12.74
ATOM	194	CD2	TYR	25	2.664	-5.252	12.087	1.00	11.55
ATOM	195	CE2	TYR	25	4.014	-5.532	12.241	1.00	12.00
ATOM	196	CZ	TYR	25	4.940	-4.516	12.148	1.00	13.06
ATOM	197	OH	TYR	25	6.286	-4.805	12.308	1.00	15.97
ATOM	198	C	TYR	25	-1.430	-4.563	10.837	1.00	9.93
ATOM	199	O	TYR	25	-1.885	-5.160	11.815	1.00	9.61
ATOM	200	N	ARG	26	-2.204	-3.934	9.956	1.00	8.48
ATOM	201	CA	ARG	26	-3.650	-3.920	10.116	1.00	10.08
ATOM	202	CB	ARG	26	-4.316	-3.139	8.980	1.00	9.99
ATOM	203	CG	ARG	26	-5.825	-3.177	9.065	1.00	9.56
ATOM	204	CD	ARG	26	-6.491	-2.185	8.134	1.00	8.61
ATOM	205	NE	ARG	26	-6.341	-2.519	6.715	1.00	10.49
ATOM	206	CZ	ARG	26	-7.004	-1.881	5.752	1.00	10.54
ATOM	207	NH1	ARG	26	-7.840	-.902	6.075	1.00	10.25
ATOM	208	NH2	ARG	26	-6.836	-2.213	4.479	1.00	12.32
ATOM	209	C	ARG	26	-4.192	-5.342	10.157	1.00	10.26
ATOM	210	O	ARG	26	-3.983	-6.121	9.235	1.00	11.08
ATOM	211	N	PRO	27	-4.922	-5.688	11.220	1.00	10.55
ATOM	212	CD	PRO	27	-5.175	-4.912	12.448	1.00	10.34
ATOM	213	CA	PRO	27	-5.464	-7.046	11.324	1.00	11.12
ATOM	214	CB	PRO	27	-5.804	-7.154	12.803	1.00	10.70
ATOM	215	CG	PRO	27	-6.201	-5.753	13.159	1.00	10.99
ATOM	216	C	PRO	27	-6.667	-7.333	10.441	1.00	12.12
ATOM	217	O	PRO	27	-6.884	-8.478	10.026	1.00	12.58
ATOM	218	N	SER	28	-7.423	-6.285	10.140	1.00	12.76
ATOM	219	CA	SER	28	-8.641	-6.401	9.359	1.00	13.44
ATOM	220	CB	SER	28	-9.783	-6.791	10.308	1.00	15.76
ATOM	221	OG	SER	28	-11.054	-6.557	9.738	1.00	16.03
ATOM	222	C	SER	28	-8.980	-5.090	8.670	1.00	13.58
ATOM	223	O	SER	28	-8.982	-4.040	9.316	1.00	12.29
ATOM	224	N	ALA	29	-9.265	-5.144	7.368	1.00	13.53
ATOM	225	CA	ALA	29	-9.650	-3.946	6.637	1.00	14.70
ATOM	226	CB	ALA	29	-9.706	-4.223	5.134	1.00	15.27
ATOM	227	C	ALA	29	-11.023	-3.521	7.130	1.00	15.68
ATOM	228	O	ALA	29	-11.340	-2.333	7.135	1.00	15.22
ATOM	229	N	GLU	30	-11.838	-4.496	7.540	1.00	16.92
ATOM	230	CA	GLU	30	-13.178	-4.197	8.030	1.00	17.37
ATOM	231	CB	GLU	30	-14.028	-5.472	8.171	1.00	21.96
ATOM	232	CG	GLU	30	-14.190	-6.272	6.894	1.00	26.66
ATOM	233	CD	GLU	30	-14.561	-5.414	5.707	1.00	28.96
ATOM	234	OE1	GLU	30	-15.594	-4.704	5.768	1.00	31.37
ATOM	235	OE2	GLU	30	-13.815	-5.436	4.704	1.00	31.46
ATOM	236	C	GLU	30	-13.137	-3.493	9.375	1.00	16.63
ATOM	237	O	GLU	30	-13.859	-2.528	9.575	1.00	15.36
ATOM	238	N	LEU	31	-12.294	-3.974	10.291	1.00	15.81
ATOM	239	CA	LEU	31	-12.185	-3.382	11.621	1.00	15.44
ATOM	240	CB	LEU	31	-11.471	-4.348	12.578	1.00	18.26
ATOM	241	CG	LEU	31	-12.280	-5.596	12.956	1.00	21.03
ATOM	242	CD1	LEU	31	-11.543	-6.458	13.961	1.00	22.31
ATOM	243	CD2	LEU	31	-13.601	-5.146	13.535	1.00	20.90
ATOM	244	C	LEU	31	-11.477	-2.036	11.648	1.00	14.02
ATOM	245	O	LEU	31	-11.803	-1.172	12.466	1.00	14.03
ATOM	246	N	PHE	32	-10.528	-1.846	10.741	1.00	11.76
ATOM	247	CA	PHE	32	-9.783	-.603	10.699	1.00	10.71
ATOM	248	CB	PHE	32	-8.365	-.816	11.229	1.00	10.30
ATOM	249	CG	PHE	32	-8.315	-1.176	12.680	1.00	10.67
ATOM	250	CD1	PHE	32	-8.332	-2.505	13.083	1.00	11.00
ATOM	251	CD2	PHE	32	-8.253	-.180	13.647	1.00	12.04
ATOM	252	CE1	PHE	32	-8.286	-2.842	14.443	1.00	12.97

ATOM	253	CE2	PHE	32	-8.205	-.506	15.004	1.00	12.19
ATOM	254	CZ	PHE	32	-8.220	-1.830	15.402	1.00	12.65
ATOM	255	C	PHE	32	-9.694	.043	9.330	1.00	9.99
ATOM	256	O	PHE	32	-8.642	.016	8.690	1.00	10.09
ATOM	257	N	PRO	33	-10.801	.633	8.858	1.00	9.96
ATOM	258	CD	PRO	33	-12.095	.838	9.524	1.00	11.05
ATOM	259	CA	PRO	33	-10.768	1.279	7.543	1.00	9.68
ATOM	260	CB	PRO	33	-12.205	1.766	7.333	1.00	10.24
ATOM	261	CG	PRO	33	-13.011	1.023	8.358	1.00	12.04
ATOM	262	C	PRO	33	-9.792	2.437	7.631	1.00	10.30
ATOM	263	O	PRO	33	-9.719	3.123	8.653	1.00	10.14
ATOM	264	N	ILE	34	-9.039	2.644	6.559	1.00	10.12
ATOM	265	CA	ILE	34	-8.063	3.716	6.523	1.00	10.17
ATOM	266	CB	ILE	34	-6.713	3.202	6.042	1.00	9.45
ATOM	267	CG2	ILE	34	-5.750	4.373	5.816	1.00	10.13
ATOM	268	CG1	ILE	34	-6.179	2.184	7.063	1.00	9.62
ATOM	269	CD1	ILE	34	-4.979	1.432	6.598	1.00	10.53
ATOM	270	C	ILE	34	-8.551	4.796	5.584	1.00	10.05
ATOM	271	O	ILE	34	-8.885	4.527	4.443	1.00	10.49
ATOM	272	N	ILE	35	-8.637	6.012	6.098	1.00	9.71
ATOM	273	CA	ILE	35	-9.071	7.146	5.296	1.00	9.38
ATOM	274	CB	ILE	35	-10.302	7.864	5.923	1.00	10.15
ATOM	275	CG2	ILE	35	-10.612	9.149	5.155	1.00	10.24
ATOM	276	CG1	ILE	35	-11.531	6.952	5.883	1.00	11.45
ATOM	277	CD1	ILE	35	-11.455	5.789	6.834	1.00	12.04
ATOM	278	C	ILE	35	-7.910	8.117	5.253	1.00	9.44
ATOM	279	O	ILE	35	-7.472	8.618	6.291	1.00	10.00
ATOM	280	N	VAL	36	-7.404	8.368	4.053	1.00	7.60
ATOM	281	CA	VAL	36	-6.307	9.293	3.871	1.00	8.52
ATOM	282	CB	VAL	36	-5.285	8.763	2.846	1.00	7.91
ATOM	283	CG1	VAL	36	-4.102	9.697	2.789	1.00	7.80
ATOM	284	CG2	VAL	36	-4.828	7.349	3.230	1.00	9.29
ATOM	285	C	VAL	36	-6.853	10.626	3.377	1.00	8.11
ATOM	286	O	VAL	36	-7.359	10.719	2.259	1.00	7.95
ATOM	287	N	SER	37	-6.788	11.643	4.231	1.00	8.27
ATOM	288	CA	SER	37	-7.241	12.973	3.850	1.00	8.72
ATOM	289	CB	SER	37	-7.896	13.682	5.035	1.00	9.04
ATOM	290	OG	SER	37	-8.289	15.000	4.682	1.00	10.03
ATOM	291	C	SER	37	-6.014	13.744	3.406	1.00	9.28
ATOM	292	O	SER	37	-5.097	13.983	4.199	1.00	9.18
ATOM	293	N	GLN	38	-5.978	14.124	2.134	1.00	9.51
ATOM	294	CA	GLN	38	-4.841	14.860	1.619	1.00	10.96
ATOM	295	CB	GLN	38	-4.346	14.265	.294	1.00	11.85
ATOM	296	CG	GLN	38	-3.042	14.910	-.216	1.00	12.23
ATOM	297	CD	GLN	38	-2.768	14.649	-1.698	1.00	12.33
ATOM	298	OE1	GLN	38	-3.457	13.862	-2.339	1.00	12.96
ATOM	299	NE2	GLN	38	-1.748	15.311	-2.239	1.00	12.38
ATOM	300	C	GLN	38	-5.219	16.299	1.377	1.00	11.49
ATOM	301	O	GLN	38	-6.232	16.583	.737	1.00	11.90
ATOM	302	N	ASP	39	-4.398	17.205	1.891	1.00	12.65
ATOM	303	CA	ASP	39	-4.594	18.632	1.704	1.00	13.36
ATOM	304	CB	ASP	39	-4.474	19.332	3.065	1.00	12.17
ATOM	305	CG	ASP	39	-4.717	20.819	2.995	1.00	12.83
ATOM	306	OD1	ASP	39	-5.414	21.282	2.063	1.00	11.15
ATOM	307	OD2	ASP	39	-4.220	21.521	3.899	1.00	13.23
ATOM	308	C	ASP	39	-3.456	19.053	.768	1.00	15.38
ATOM	309	O	ASP	39	-2.624	18.214	.394	1.00	15.95
ATOM	310	N	CYS	40	-3.441	20.321	.356	1.00	16.65
ATOM	311	CA	CYS	40	-2.368	20.861	-.491	1.00	18.96
ATOM	312	C	CYS	40	-2.337	20.569	-1.990	1.00	19.46

ATOM	313	O	CYS	40	-1.646	21.266	-2.741	1.00	20.24
ATOM	314	CB	CYS	40	-1.025	20.462	.099	1.00	20.44
ATOM	315	SG	CYS	40	-.982	20.733	1.876	1.00	23.33
ATOM	316	N	GLY	41	-3.062	19.550	-2.434	1.00	20.37
ATOM	317	CA	GLY	41	-3.079	19.227	-3.856	1.00	20.72
ATOM	318	C	GLY	41	-1.713	18.957	-4.476	1.00	20.47
ATOM	319	O	GLY	41	-1.453	19.358	-5.609	1.00	21.24
ATOM	320	N	HIS	42	-.829	18.293	-3.741	1.00	19.60
ATOM	321	CA	HIS	42	.506	17.960	-4.242	1.00	19.16
ATOM	322	CB	HIS	42	1.445	17.743	-3.045	1.00	18.66
ATOM	323	CG	HIS	42	2.846	17.370	-3.422	1.00	18.14
ATOM	324	CD2	HIS	42	3.956	18.128	-3.593	1.00	18.57
ATOM	325	ND1	HIS	42	3.229	16.070	-3.659	1.00	17.40
ATOM	326	CE1	HIS	42	4.515	16.038	-3.956	1.00	18.21
ATOM	327	NE2	HIS	42	4.981	17.274	-3.923	1.00	18.29
ATOM	328	C	HIS	42	.307	16.690	-5.074	1.00	20.48
ATOM	329	O	HIS	42	.016	15.615	-4.536	1.00	18.37
ATOM	330	N	GLU	43	.440	16.823	-6.395	1.00	22.05
ATOM	331	CA	GLU	43	.185	15.716	-7.315	1.00	22.74
ATOM	332	CB	GLU	43	.333	16.203	-8.761	1.00	26.75
ATOM	333	CG	GLU	43	-.569	15.476	-9.756	1.00	29.70
ATOM	334	CD	GLU	43	-2.038	15.472	-9.334	1.00	31.48
ATOM	335	OE1	GLU	43	-2.535	16.531	-8.874	1.00	32.26
ATOM	336	OE2	GLU	43	-2.709	14.425	-9.478	1.00	32.29
ATOM	337	C	GLU	43	.949	14.408	-7.132	1.00	22.76
ATOM	338	O	GLU	43	.354	13.333	-7.231	1.00	21.67
ATOM	339	N	GLU	44	2.252	14.475	-6.888	1.00	23.45
ATOM	340	CA	GLU	44	3.027	13.253	-6.708	1.00	23.36
ATOM	341	CB	GLU	44	4.486	13.606	-6.424	1.00	28.28
ATOM	342	CG	GLU	44	5.418	12.429	-6.295	1.00	33.72
ATOM	343	CD	GLU	44	6.881	12.854	-6.188	1.00	36.47
ATOM	344	OE1	GLU	44	7.764	11.974	-6.121	1.00	38.34
ATOM	345	OE2	GLU	44	7.169	14.070	-6.172	1.00	38.85
ATOM	346	C	GLU	44	2.442	12.451	-5.540	1.00	22.01
ATOM	347	O	GLU	44	2.308	11.219	-5.601	1.00	21.23
ATOM	348	N	THR	45	2.090	13.158	-4.475	1.00	19.27
ATOM	349	CA	THR	45	1.537	12.510	-3.298	1.00	16.93
ATOM	350	CB	THR	45	1.422	13.510	-2.132	1.00	16.06
ATOM	351	OG1	THR	45	2.720	14.041	-1.827	1.00	16.03
ATOM	352	CG2	THR	45	.866	12.818	-.897	1.00	16.75
ATOM	353	C	THR	45	.164	11.921	-3.600	1.00	16.17
ATOM	354	O	THR	45	-.185	10.838	-3.105	1.00	15.51
ATOM	355	N	ALA	46	-.614	12.640	-4.401	1.00	15.60
ATOM	356	CA	ALA	46	-1.955	12.207	-4.776	1.00	15.63
ATOM	357	CB	ALA	46	-2.625	13.270	-5.624	1.00	15.81
ATOM	358	C	ALA	46	-1.846	10.903	-5.553	1.00	16.79
ATOM	359	O	ALA	46	-2.615	9.965	-5.338	1.00	15.70
ATOM	360	N	GLN	47	-.879	10.857	-6.469	1.00	17.63
ATOM	361	CA	GLN	47	-.640	9.659	-7.254	1.00	18.02
ATOM	362	CB	GLN	47	.397	9.952	-8.341	1.00	22.53
ATOM	363	CG	GLN	47	-.206	10.723	-9.528	1.00	26.91
ATOM	364	CD	GLN	47	.758	11.691	-10.192	1.00	29.92
ATOM	365	OE1	GLN	47	1.823	11.306	-10.702	1.00	31.99
ATOM	366	NE2	GLN	47	.384	12.965	-10.194	1.00	31.40
ATOM	367	C	GLN	47	-.190	8.507	-6.351	1.00	16.72
ATOM	368	O	GLN	47	-.612	7.371	-6.526	1.00	16.34
ATOM	369	N	VAL	48	.660	8.789	-5.377	1.00	15.54
ATOM	370	CA	VAL	48	1.099	7.735	-4.474	1.00	14.29
ATOM	371	CB	VAL	48	2.189	8.252	-3.490	1.00	14.08
ATOM	372	CG1	VAL	48	2.453	7.220	-2.403	1.00	14.73

ATOM	373	CG2	VAL	48	3.484	8.537	-4.250	1.00	15.17
ATOM	374	C	VAL	48	-.084	7.159	-3.690	1.00	13.70
ATOM	375	O	VAL	48	-.259	5.943	-3.623	1.00	13.68
ATOM	376	N	ILE	49	-.913	8.026	-3.118	1.00	12.75
ATOM	377	CA	ILE	49	-2.054	7.552	-2.346	1.00	12.65
ATOM	378	CB	ILE	49	-2.814	8.738	-1.672	1.00	11.26
ATOM	379	CG2	ILE	49	-4.013	8.223	-.880	1.00	12.06
ATOM	380	CG1	ILE	49	-1.863	9.481	-.717	1.00	11.68
ATOM	381	CD1	ILE	49	-2.388	10.803	-.186	1.00	11.25
ATOM	382	C	ILE	49	-2.999	6.748	-3.225	1.00	12.59
ATOM	383	O	ILE	49	-3.418	5.648	-2.857	1.00	12.18
ATOM	384	N	ALA	50	-3.305	7.281	-4.405	1.00	12.93
ATOM	385	CA	ALA	50	-4.210	6.628	-5.338	1.00	13.31
ATOM	386	CB	ALA	50	-4.370	7.498	-6.583	1.00	12.34
ATOM	387	C	ALA	50	-3.751	5.223	-5.740	1.00	13.06
ATOM	388	O	ALA	50	-4.577	4.347	-5.971	1.00	13.74
ATOM	389	N	SER	51	-2.438	4.997	-5.790	1.00	13.74
ATOM	390	CA	SER	51	-1.927	3.694	-6.199	1.00	13.55
ATOM	391	CB	SER	51	-.418	3.775	-6.456	1.00	12.32
ATOM	392	OG	SER	51	.317	3.810	-5.245	1.00	14.44
ATOM	393	C	SER	51	-2.227	2.540	-5.238	1.00	13.38
ATOM	394	O	SER	51	-1.984	1.383	-5.575	1.00	14.73
ATOM	395	N	TYR	52	-2.720	2.841	-4.037	1.00	12.07
ATOM	396	CA	TYR	52	-3.057	1.787	-3.077	1.00	11.68
ATOM	397	CB	TYR	52	-3.035	2.326	-1.640	1.00	10.89
ATOM	398	CG	TYR	52	-1.639	2.549	-1.107	1.00	11.23
ATOM	399	CD1	TYR	52	-.888	3.662	-1.498	1.00	11.20
ATOM	400	CE1	TYR	52	.403	3.860	-1.028	1.00	10.93
ATOM	401	CD2	TYR	52	-1.056	1.632	-.232	1.00	10.99
ATOM	402	CE2	TYR	52	.240	1.818	.238	1.00	11.45
ATOM	403	CZ	TYR	52	.961	2.940	-.166	1.00	10.39
ATOM	404	OH	TYR	52	2.237	3.155	.308	1.00	11.63
ATOM	405	C	TYR	52	-4.449	1.270	-3.399	1.00	12.25
ATOM	406	O	TYR	52	-4.920	.291	-2.821	1.00	12.40
ATOM	407	N	GLY	53	-5.102	1.949	-4.334	1.00	12.71
ATOM	408	CA	GLY	53	-6.433	1.567	-4.731	1.00	13.02
ATOM	409	C	GLY	53	-7.383	1.511	-3.565	1.00	13.52
ATOM	410	O	GLY	53	-7.397	2.408	-2.704	1.00	13.34
ATOM	411	N	SER	54	-8.166	.439	-3.538	1.00	13.99
ATOM	412	CA	SER	54	-9.179	.211	-2.507	1.00	13.99
ATOM	413	CB	SER	54	-10.109	-.927	-2.942	1.00	14.52
ATOM	414	OG	SER	54	-9.400	-2.155	-3.072	1.00	15.92
ATOM	415	C	SER	54	-8.645	-.087	-1.111	1.00	13.53
ATOM	416	O	SER	54	-9.425	-.189	-.158	1.00	13.36
ATOM	417	N	ALA	55	-7.333	-.244	-.980	1.00	12.77
ATOM	418	CA	ALA	55	-6.764	-.534	.328	1.00	12.60
ATOM	419	CB	ALA	55	-5.261	-.769	.215	1.00	11.23
ATOM	420	C	ALA	55	-7.052	.615	1.293	1.00	12.08
ATOM	421	O	ALA	55	-7.088	.413	2.504	1.00	11.86
ATOM	422	N	VAL	56	-7.264	1.808	.743	1.00	11.93
ATOM	423	CA	VAL	56	-7.571	3.009	1.530	1.00	11.80
ATOM	424	CB	VAL	56	-6.326	3.931	1.716	1.00	11.86
ATOM	425	CG1	VAL	56	-5.197	3.188	2.401	1.00	11.85
ATOM	426	CG2	VAL	56	-5.872	4.470	.365	1.00	13.56
ATOM	427	C	VAL	56	-8.624	3.840	.797	1.00	12.23
ATOM	428	O	VAL	56	-8.933	3.565	-.357	1.00	12.80
ATOM	429	N	THR	57	-9.188	4.841	1.474	1.00	11.34
ATOM	430	CA	THR	57	-10.149	5.740	.840	1.00	11.96
ATOM	431	CB	THR	57	-11.481	5.880	1.623	1.00	12.67
ATOM	432	OG1	THR	57	-12.114	4.600	1.746	1.00	14.47

ATOM	433	CG2	THR	57	-12.425	6.820	.865	1.00	12.73
ATOM	434	C	THR	57	-9.443	7.099	.825	1.00	11.95
ATOM	435	O	THR	57	-9.065	7.623	1.872	1.00	12.82
ATOM	436	N	HIS	58	-9.265	7.656	-.368	1.00	11.73
ATOM	437	CA	HIS	58	-8.562	8.921	-.551	1.00	11.93
ATOM	438	CB	HIS	58	-7.700	8.791	-1.823	1.00	11.77
ATOM	439	CG	HIS	58	-6.796	9.955	-2.090	1.00	12.34
ATOM	440	CD2	HIS	58	-6.413	10.996	-1.311	1.00	12.55
ATOM	441	ND1	HIS	58	-6.150	10.123	-3.300	1.00	12.61
ATOM	442	CE1	HIS	58	-5.413	11.218	-3.253	1.00	13.06
ATOM	443	NE2	HIS	58	-5.554	11.767	-2.058	1.00	12.93
ATOM	444	C	HIS	58	-9.545	10.086	-.678	1.00	11.57
ATOM	445	O	HIS	58	-10.349	10.103	-1.604	1.00	12.49
ATOM	446	N	ILE	59	-9.503	11.039	.255	1.00	10.72
ATOM	447	CA	ILE	59	-10.379	12.208	.185	1.00	10.48
ATOM	448	CB	ILE	59	-11.337	12.299	1.396	1.00	10.13
ATOM	449	CG2	ILE	59	-12.209	11.038	1.463	1.00	10.25
ATOM	450	CG1	ILE	59	-10.552	12.444	2.703	1.00	9.21
ATOM	451	CD1	ILE	59	-11.447	12.671	3.941	1.00	10.09
ATOM	452	C	ILE	59	-9.488	13.446	.109	1.00	11.16
ATOM	453	O	ILE	59	-8.345	13.425	.570	1.00	9.86
ATOM	454	N	ARG	60	-9.998	14.523	-.478	1.00	12.11
ATOM	455	CA	ARG	60	-9.193	15.724	-.657	1.00	12.88
ATOM	456	CB	ARG	60	-8.946	15.939	-2.148	1.00	16.27
ATOM	457	CG	ARG	60	-8.447	14.696	-2.867	1.00	20.66
ATOM	458	CD	ARG	60	-8.400	14.919	-4.374	1.00	25.16
ATOM	459	NE	ARG	60	-7.874	13.742	-5.055	1.00	29.56
ATOM	460	CZ	ARG	60	-8.585	12.669	-5.389	1.00	32.13
ATOM	461	NH1	ARG	60	-9.891	12.595	-5.121	1.00	33.70
ATOM	462	NH2	ARG	60	-7.968	11.648	-5.969	1.00	33.58
ATOM	463	C	ARG	60	-9.753	17.010	-.067	1.00	12.02
ATOM	464	O	ARG	60	-10.857	17.442	-.422	1.00	12.79
ATOM	465	N	GLN	61	-8.989	17.636	.821	1.00	10.88
ATOM	466	CA	GLN	61	-9.444	18.887	1.412	1.00	10.41
ATOM	467	CB	GLN	61	-8.380	19.447	2.353	1.00	9.95
ATOM	468	CG	GLN	61	-8.928	20.461	3.333	1.00	9.31
ATOM	469	CD	GLN	61	-9.135	21.824	2.710	1.00	9.41
ATOM	470	OE1	GLN	61	-10.263	22.309	2.608	1.00	10.18
ATOM	471	NE2	GLN	61	-8.044	22.454	2.297	1.00	8.53
ATOM	472	C	GLN	61	-9.719	19.812	.212	1.00	10.78
ATOM	473	O	GLN	61	-8.828	20.085	-.591	1.00	10.46
ATOM	474	N	PRO	62	-10.961	20.309	.089	1.00	12.33
ATOM	475	CD	PRO	62	-12.091	19.994	.984	1.00	12.11
ATOM	476	CA	PRO	62	-11.393	21.177	-1.018	1.00	13.40
ATOM	477	CB	PRO	62	-12.921	21.078	-.946	1.00	12.80
ATOM	478	CG	PRO	62	-13.171	20.958	.543	1.00	13.28
ATOM	479	C	PRO	62	-10.937	22.614	-1.188	1.00	14.06
ATOM	480	O	PRO	62	-10.858	23.094	-2.323	1.00	14.68
ATOM	481	N	ASP	63	-10.659	23.302	-.091	1.00	13.74
ATOM	482	CA	ASP	63	-10.268	24.711	-.130	1.00	15.02
ATOM	483	CB	ASP	63	-10.917	25.413	1.053	1.00	16.46
ATOM	484	CG	ASP	63	-11.091	26.891	.824	1.00	18.17
ATOM	485	OD1	ASP	63	-10.295	27.459	.051	1.00	18.42
ATOM	486	OD2	ASP	63	-12.011	27.484	1.435	1.00	18.48
ATOM	487	C	ASP	63	-8.758	24.910	-.080	1.00	15.38
ATOM	488	O	ASP	63	-8.176	24.852	.990	1.00	14.86
ATOM	489	N	LEU	64	-8.127	25.162	-1.222	1.00	16.45
ATOM	490	CA	LEU	64	-6.677	25.341	-1.250	1.00	16.76
ATOM	491	CB	LEU	64	-6.082	24.700	-2.513	1.00	18.73
ATOM	492	CG	LEU	64	-6.334	23.213	-2.795	1.00	19.87

ATOM	493	CD1	LEU	64	-7.823	22.909	-2.841	1.00	21.13
ATOM	494	CD2	LEU	64	-5.703	22.857	-4.146	1.00	20.19
ATOM	495	C	LEU	64	-6.252	26.813	-1.186	1.00	16.97
ATOM	496	O	LEU	64	-5.070	27.141	-1.372	1.00	17.71
ATOM	497	N	SER	65	-7.206	27.695	-.914	1.00	16.41
ATOM	498	CA	SER	65	-6.908	29.117	-.854	1.00	16.79
ATOM	499	CB	SER	65	-8.217	29.897	-.835	1.00	16.54
ATOM	500	OG	SER	65	-8.836	29.737	.425	1.00	16.09
ATOM	501	C	SER	65	-6.074	29.529	.364	1.00	17.63
ATOM	502	O	SER	65	-6.046	28.840	1.396	1.00	16.40
ATOM	503	N	ASN	66	-5.413	30.674	.243	1.00	18.41
ATOM	504	CA	ASN	66	-4.604	31.217	1.323	1.00	19.02
ATOM	505	CB	ASN	66	-3.726	32.365	.811	1.00	23.72
ATOM	506	CG	ASN	66	-2.726	32.832	1.849	1.00	27.27
ATOM	507	OD1	ASN	66	-1.863	32.059	2.268	1.00	29.21
ATOM	508	ND2	ASN	66	-2.840	34.089	2.283	1.00	28.68
ATOM	509	C	ASN	66	-5.579	31.738	2.373	1.00	18.59
ATOM	510	O	ASN	66	-6.678	32.202	2.044	1.00	17.29
ATOM	511	N	ILE	67	-5.182	31.647	3.637	1.00	16.84
ATOM	512	CA	ILE	67	-6.020	32.081	4.747	1.00	16.42
ATOM	513	CB	ILE	67	-6.003	31.021	5.889	1.00	16.04
ATOM	514	CG2	ILE	67	-6.816	31.513	7.083	1.00	17.81
ATOM	515	CG1	ILE	67	-6.568	29.690	5.368	1.00	16.60
ATOM	516	CD1	ILE	67	-6.246	28.490	6.271	1.00	15.88
ATOM	517	C	ILE	67	-5.515	33.410	5.290	1.00	15.92
ATOM	518	O	ILE	67	-4.301	33.622	5.405	1.00	16.68
ATOM	519	N	ALA	68	-6.449	34.303	5.613	1.00	15.43
ATOM	520	CA	ALA	68	-6.106	35.607	6.164	1.00	14.99
ATOM	521	CB	ALA	68	-7.300	36.532	6.089	1.00	14.38
ATOM	522	C	ALA	68	-5.721	35.348	7.611	1.00	13.82
ATOM	523	O	ALA	68	-6.495	34.748	8.369	1.00	15.04
ATOM	524	N	VAL	69	-4.521	35.773	7.987	1.00	12.64
ATOM	525	CA	VAL	69	-4.027	35.574	9.353	1.00	11.52
ATOM	526	CB	VAL	69	-2.555	35.065	9.365	1.00	11.38
ATOM	527	CG1	VAL	69	-2.417	33.809	8.491	1.00	11.77
ATOM	528	CG2	VAL	69	-1.611	36.148	8.863	1.00	10.86
ATOM	529	C	VAL	69	-4.103	36.853	10.173	1.00	11.07
ATOM	530	O	VAL	69	-4.224	37.946	9.621	1.00	10.98
ATOM	531	N	GLN	70	-4.032	36.717	11.494	1.00	10.25
ATOM	532	CA	GLN	70	-4.080	37.885	12.369	1.00	9.22
ATOM	533	CB	GLN	70	-4.474	37.472	13.786	1.00	8.85
ATOM	534	CG	GLN	70	-5.967	37.186	13.919	1.00	11.72
ATOM	535	CD	GLN	70	-6.816	38.424	13.692	1.00	11.71
ATOM	536	OE1	GLN	70	-6.863	39.329	14.534	1.00	11.62
ATOM	537	NE2	GLN	70	-7.490	38.476	12.546	1.00	13.16
ATOM	538	C	GLN	70	-2.716	38.559	12.351	1.00	9.55
ATOM	539	O	GLN	70	-1.731	37.950	11.957	1.00	10.19
ATOM	540	N	PRO	71	-2.643	39.824	12.794	1.00	10.05
ATOM	541	CD	PRO	71	-3.749	40.603	13.379	1.00	10.73
ATOM	542	CA	PRO	71	-1.396	40.599	12.811	1.00	10.56
ATOM	543	CB	PRO	71	-1.808	41.913	13.468	1.00	10.79
ATOM	544	CG	PRO	71	-3.261	42.008	13.188	1.00	9.90
ATOM	545	C	PRO	71	-.170	40.014	13.484	1.00	10.60
ATOM	546	O	PRO	71	.952	40.442	13.197	1.00	11.80
ATOM	547	N	ASP	72	-.364	39.060	14.384	1.00	10.85
ATOM	548	CA	ASP	72	.778	38.471	15.078	1.00	10.30
ATOM	549	CB	ASP	72	.415	38.186	16.549	1.00	11.30
ATOM	550	CG	ASP	72	-.850	37.350	16.699	1.00	11.31
ATOM	551	OD1	ASP	72	-1.725	37.413	15.802	1.00	10.03
ATOM	552	OD2	ASP	72	-.979	36.634	17.725	1.00	11.28

ATOM	553	C	ASP	72	1.227	37.186	14.407	1.00	10.88
ATOM	554	O	ASP	72	2.155	36.536	14.877	1.00	10.58
ATOM	555	N	HIS	73	.597	36.842	13.287	1.00	11.05
ATOM	556	CA	HIS	73	.892	35.564	12.632	1.00	12.10
ATOM	557	CB	HIS	73	-.326	34.650	12.782	1.00	11.18
ATOM	558	CG	HIS	73	-.652	34.293	14.197	1.00	10.79
ATOM	559	CD2	HIS	73	.134	34.153	15.291	1.00	9.83
ATOM	560	ND1	HIS	73	-1.927	33.945	14.593	1.00	10.24
ATOM	561	CE1	HIS	73	-1.909	33.598	15.867	1.00	10.32
ATOM	562	NE2	HIS	73	-.671	33.715	16.315	1.00	10.28
ATOM	563	C	HIS	73	1.320	35.535	11.167	1.00	13.40
ATOM	564	O	HIS	73	1.027	34.559	10.465	1.00	12.54
ATOM	565	N	ARG	74	2.001	36.570	10.692	1.00	15.07
ATOM	566	CA	ARG	74	2.445	36.562	9.295	1.00	17.32
ATOM	567	CB	ARG	74	3.225	37.840	8.970	1.00	20.87
ATOM	568	CG	ARG	74	2.367	38.952	8.419	1.00	25.78
ATOM	569	CD	ARG	74	1.815	38.620	7.034	1.00	30.08
ATOM	570	NE	ARG	74	.666	39.472	6.746	1.00	34.64
ATOM	571	CZ	ARG	74	-.167	39.322	5.721	1.00	37.24
ATOM	572	NH1	ARG	74	.018	38.341	4.840	1.00	38.96
ATOM	573	NH2	ARG	74	-1.224	40.130	5.610	1.00	38.72
ATOM	574	C	ARG	74	3.320	35.355	8.981	1.00	17.59
ATOM	575	O	ARG	74	3.265	34.812	7.871	1.00	17.32
ATOM	576	N	LYS	75	4.130	34.942	9.954	1.00	17.56
ATOM	577	CA	LYS	75	5.039	33.806	9.780	1.00	17.68
ATOM	578	CB	LYS	75	6.153	33.832	10.840	1.00	19.54
ATOM	579	CG	LYS	75	7.006	35.083	10.963	1.00	21.50
ATOM	580	CD	LYS	75	7.906	34.916	12.175	1.00	22.78
ATOM	581	CE	LYS	75	9.227	35.644	12.039	1.00	24.28
ATOM	582	NZ	LYS	75	10.138	35.215	13.147	1.00	25.07
ATOM	583	C	LYS	75	4.360	32.439	9.911	1.00	17.66
ATOM	584	O	LYS	75	5.003	31.407	9.693	1.00	17.69
ATOM	585	N	PHE	76	3.073	32.413	10.243	1.00	15.60
ATOM	586	CA	PHE	76	2.419	31.141	10.485	1.00	15.31
ATOM	587	CB	PHE	76	2.007	31.115	11.956	1.00	15.06
ATOM	588	CG	PHE	76	3.125	31.482	12.885	1.00	15.46
ATOM	589	CD1	PHE	76	3.146	32.713	13.540	1.00	15.79
ATOM	590	CD2	PHE	76	4.207	30.617	13.051	1.00	15.61
ATOM	591	CE1	PHE	76	4.234	33.078	14.344	1.00	15.44
ATOM	592	CE2	PHE	76	5.302	30.969	13.851	1.00	16.15
ATOM	593	CZ	PHE	76	5.319	32.197	14.497	1.00	15.86
ATOM	594	C	PHE	76	1.275	30.650	9.603	1.00	15.24
ATOM	595	O	PHE	76	.422	29.902	10.070	1.00	14.94
ATOM	596	N	GLN	77	1.284	31.024	8.326	1.00	15.76
ATOM	597	CA	GLN	77	.256	30.574	7.392	1.00	15.39
ATOM	598	CB	GLN	77	.637	30.965	5.957	1.00	17.04
ATOM	599	CG	GLN	77	-.279	30.368	4.889	1.00	19.15
ATOM	600	CD	GLN	77	-1.690	30.947	4.928	1.00	20.46
ATOM	601	OE1	GLN	77	-2.675	30.283	4.551	1.00	21.18
ATOM	602	NE2	GLN	77	-1.797	32.193	5.363	1.00	20.79
ATOM	603	C	GLN	77	.048	29.049	7.465	1.00	15.06
ATOM	604	O	GLN	77	-1.089	28.562	7.505	1.00	13.55
ATOM	605	N	GLY	78	1.154	28.307	7.490	1.00	13.38
ATOM	606	CA	GLY	78	1.097	26.852	7.530	1.00	13.54
ATOM	607	C	GLY	78	.290	26.296	8.682	1.00	13.51
ATOM	608	O	GLY	78	-.408	25.285	8.523	1.00	13.11
ATOM	609	N	TYR	79	.391	26.940	9.844	1.00	11.80
ATOM	610	CA	TYR	79	-.359	26.489	11.014	1.00	11.83
ATOM	611	CB	TYR	79	.154	27.157	12.286	1.00	12.65
ATOM	612	CG	TYR	79	1.446	26.562	12.771	1.00	15.02

ATOM	613	CD1	TYR	79	2.674	27.133	12.441	1.00	15.85
ATOM	614	CE1	TYR	79	3.879	26.565	12.887	1.00	17.32
ATOM	615	CD2	TYR	79	1.439	25.406	13.557	1.00	15.74
ATOM	616	CE2	TYR	79	2.635	24.827	14.007	1.00	17.18
ATOM	617	CZ	TYR	79	3.847	25.413	13.666	1.00	17.65
ATOM	618	OH	TYR	79	5.025	24.828	14.088	1.00	18.77
ATOM	619	C	TYR	79	-1.856	26.749	10.848	1.00	11.17
ATOM	620	O	TYR	79	-2.676	26.021	11.412	1.00	11.44
ATOM	621	N	TYR	80	-2.215	27.790	10.096	1.00	10.34
ATOM	622	CA	TYR	80	-3.622	28.070	9.840	1.00	8.67
ATOM	623	CB	TYR	80	-3.818	29.458	9.196	1.00	8.12
ATOM	624	CG	TYR	80	-3.851	30.621	10.165	1.00	7.91
ATOM	625	CD1	TYR	80	-2.706	31.013	10.858	1.00	8.01
ATOM	626	CE1	TYR	80	-2.722	32.122	11.708	1.00	8.25
ATOM	627	CD2	TYR	80	-5.018	31.362	10.351	1.00	7.69
ATOM	628	CE2	TYR	80	-5.046	32.484	11.205	1.00	8.21
ATOM	629	CZ	TYR	80	-3.890	32.849	11.874	1.00	8.87
ATOM	630	OH	TYR	80	-3.884	33.936	12.724	1.00	9.27
ATOM	631	C	TYR	80	-4.168	26.995	8.882	1.00	9.35
ATOM	632	O	TYR	80	-5.299	26.517	9.036	1.00	9.49
ATOM	633	N	LYS	81	-3.371	26.629	7.878	1.00	9.62
ATOM	634	CA	LYS	81	-3.797	25.604	6.928	1.00	10.47
ATOM	635	CB	LYS	81	-2.806	25.491	5.759	1.00	12.29
ATOM	636	CG	LYS	81	-2.855	26.694	4.804	1.00	15.67
ATOM	637	CD	LYS	81	-1.942	26.550	3.590	1.00	17.38
ATOM	638	CE	LYS	81	-2.262	27.636	2.540	1.00	19.39
ATOM	639	NZ	LYS	81	-1.369	27.582	1.332	1.00	21.66
ATOM	640	C	LYS	81	-3.972	24.244	7.612	1.00	9.85
ATOM	641	O	LYS	81	-4.929	23.530	7.322	1.00	9.47
ATOM	642	N	ILE	82	-3.066	23.892	8.527	1.00	9.29
ATOM	643	CA	ILE	82	-3.164	22.616	9.230	1.00	9.63
ATOM	644	CB	ILE	82	-1.918	22.355	10.116	1.00	10.30
ATOM	645	CG2	ILE	82	-2.089	21.044	10.882	1.00	11.14
ATOM	646	CG1	ILE	82	-.666	22.275	9.236	1.00	10.59
ATOM	647	CD1	ILE	82	.648	22.247	10.017	1.00	10.32
ATOM	648	C	ILE	82	-4.439	22.584	10.089	1.00	9.78
ATOM	649	O	ILE	82	-5.137	21.559	10.153	1.00	9.59
ATOM	650	N	ALA	83	-4.761	23.702	10.739	1.00	8.86
ATOM	651	CA	ALA	83	-5.975	23.730	11.558	1.00	8.00
ATOM	652	CB	ALA	83	-6.052	25.035	12.365	1.00	8.21
ATOM	653	C	ALA	83	-7.213	23.570	10.669	1.00	8.16
ATOM	654	O	ALA	83	-8.163	22.882	11.035	1.00	8.48
ATOM	655	N	ARG	84	-7.208	24.207	9.499	1.00	7.08
ATOM	656	CA	ARG	84	-8.342	24.082	8.578	1.00	7.52
ATOM	657	CB	ARG	84	-8.146	24.980	7.346	1.00	8.92
ATOM	658	CG	ARG	84	-9.221	24.784	6.265	1.00	9.50
ATOM	659	CD	ARG	84	-9.091	25.798	5.126	1.00	9.84
ATOM	660	NE	ARG	84	-7.811	25.681	4.436	1.00	10.23
ATOM	661	CZ	ARG	84	-7.373	26.539	3.518	1.00	10.90
ATOM	662	NH1	ARG	84	-8.115	27.585	3.171	1.00	10.51
ATOM	663	NH2	ARG	84	-6.187	26.352	2.951	1.00	10.83
ATOM	664	C	ARG	84	-8.498	22.633	8.109	1.00	7.50
ATOM	665	O	ARG	84	-9.614	22.106	8.034	1.00	7.94
ATOM	666	N	HIS	85	-7.376	22.005	7.768	1.00	8.03
ATOM	667	CA	HIS	85	-7.386	20.624	7.288	1.00	8.10
ATOM	668	CB	HIS	85	-5.965	20.186	6.913	1.00	7.63
ATOM	669	CG	HIS	85	-5.904	18.837	6.264	1.00	7.28
ATOM	670	CD2	HIS	85	-6.866	18.084	5.680	1.00	7.86
ATOM	671	ND1	HIS	85	-4.735	18.117	6.153	1.00	9.20
ATOM	672	CE1	HIS	85	-4.980	16.975	5.532	1.00	8.92

ATOM	673	NE2	HIS	85	-6.264	16.933	5.232	1.00	7.35
ATOM	674	C	HIS	85	-7.967	19.680	8.346	1.00	8.22
ATOM	675	O	HIS	85	-8.834	18.859	8.044	1.00	8.04
ATOM	676	N	TYR	86	-7.507	19.815	9.589	1.00	8.97
ATOM	677	CA	TYR	86	-8.009	18.976	10.676	1.00	9.37
ATOM	678	CB	TYR	86	-7.334	19.331	12.003	1.00	9.77
ATOM	679	CG	TYR	86	-6.127	18.481	12.310	1.00	9.99
ATOM	680	CD1	TYR	86	-4.948	18.632	11.595	1.00	10.44
ATOM	681	CE1	TYR	86	-3.859	17.812	11.831	1.00	11.16
ATOM	682	CD2	TYR	86	-6.185	17.485	13.284	1.00	10.10
ATOM	683	CE2	TYR	86	-5.098	16.661	13.533	1.00	10.87
ATOM	684	CZ	TYR	86	-3.938	16.824	12.804	1.00	10.64
ATOM	685	OH	TYR	86	-2.861	16.009	13.053	1.00	10.81
ATOM	686	C	TYR	86	-9.506	19.154	10.829	1.00	10.09
ATOM	687	O	TYR	86	-10.239	18.183	10.960	1.00	9.11
ATOM	688	N	ARG	87	-9.961	20.401	10.816	1.00	11.13
ATOM	689	CA	ARG	87	-11.384	20.681	10.959	1.00	12.01
ATOM	690	CB	ARG	87	-11.626	22.190	10.935	1.00	16.48
ATOM	691	CG	ARG	87	-13.059	22.582	11.244	1.00	21.16
ATOM	692	CD	ARG	87	-13.321	24.043	10.884	1.00	25.13
ATOM	693	NE	ARG	87	-14.723	24.412	11.113	1.00	31.13
ATOM	694	CZ	ARG	87	-15.238	25.626	10.897	1.00	33.54
ATOM	695	NH1	ARG	87	-14.468	26.618	10.444	1.00	35.20
ATOM	696	NH2	ARG	87	-16.534	25.847	11.128	1.00	35.56
ATOM	697	C	ARG	87	-12.171	20.003	9.838	1.00	11.31
ATOM	698	O	ARG	87	-13.211	19.383	10.081	1.00	10.87
ATOM	699	N	TRP	88	-11.665	20.097	8.614	1.00	9.54
ATOM	700	CA	TRP	88	-12.356	19.483	7.493	1.00	9.29
ATOM	701	CB	TRP	88	-11.775	19.968	6.164	1.00	9.00
ATOM	702	CG	TRP	88	-12.495	19.386	4.984	1.00	9.68
ATOM	703	CD2	TRP	88	-12.120	18.226	4.234	1.00	10.51
ATOM	704	CE2	TRP	88	-13.110	18.029	3.241	1.00	11.19
ATOM	705	CE3	TRP	88	-11.046	17.330	4.304	1.00	10.55
ATOM	706	CD1	TRP	88	-13.666	19.831	4.436	1.00	11.21
ATOM	707	NE1	TRP	88	-14.041	19.024	3.385	1.00	10.83
ATOM	708	CZ2	TRP	88	-13.053	16.971	2.322	1.00	11.55
ATOM	709	CZ3	TRP	88	-10.991	16.273	3.392	1.00	11.83
ATOM	710	CH2	TRP	88	-11.986	16.105	2.416	1.00	11.12
ATOM	711	C	TRP	88	-12.315	17.959	7.524	1.00	9.61
ATOM	712	O	TRP	88	-13.345	17.309	7.362	1.00	9.85
ATOM	713	N	ALA	89	-11.128	17.392	7.735	1.00	9.74
ATOM	714	CA	ALA	89	-10.969	15.933	7.768	1.00	9.39
ATOM	715	CB	ALA	89	-9.471	15.564	7.868	1.00	8.39
ATOM	716	C	ALA	89	-11.749	15.289	8.912	1.00	9.17
ATOM	717	O	ALA	89	-12.361	14.239	8.733	1.00	8.66
ATOM	718	N	LEU	90	-11.724	15.895	10.092	1.00	9.17
ATOM	719	CA	LEU	90	-12.474	15.323	11.210	1.00	8.80
ATOM	720	CB	LEU	90	-12.097	16.006	12.527	1.00	10.00
ATOM	721	CG	LEU	90	-10.708	15.618	13.063	1.00	9.92
ATOM	722	CD1	LEU	90	-10.374	16.473	14.292	1.00	12.51
ATOM	723	CD2	LEU	90	-10.672	14.136	13.411	1.00	11.34
ATOM	724	C	LEU	90	-13.967	15.468	10.939	1.00	9.33
ATOM	725	O	LEU	90	-14.765	14.640	11.365	1.00	9.24
ATOM	726	N	GLY	91	-14.340	16.522	10.217	1.00	10.14
ATOM	727	CA	GLY	91	-15.741	16.717	9.883	1.00	11.04
ATOM	728	C	GLY	91	-16.171	15.583	8.970	1.00	10.93
ATOM	729	O	GLY	91	-17.259	15.036	9.105	1.00	11.99
ATOM	730	N	GLN	92	-15.306	15.221	8.030	1.00	10.45
ATOM	731	CA	GLN	92	-15.607	14.122	7.112	1.00	10.66
ATOM	732	CB	GLN	92	-14.499	13.999	6.067	1.00	12.62

ATOM	733	CG	GLN	92	-14.462	15.149	5.083	1.00	15.12
ATOM	734	CD	GLN	92	-15.657	15.132	4.141	1.00	16.27
ATOM	735	OE1	GLN	92	-15.908	14.136	3.458	1.00	18.12
ATOM	736	NE2	GLN	92	-16.390	16.231	4.094	1.00	17.52
ATOM	737	C	GLN	92	-15.762	12.775	7.816	1.00	11.46
ATOM	738	O	GLN	92	-16.722	12.033	7.579	1.00	11.11
ATOM	739	N	ILE	93	-14.821	12.445	8.692	1.00	11.19
ATOM	740	CA	ILE	93	-14.911	11.145	9.344	1.00	11.94
ATOM	741	CB	ILE	93	-13.567	10.772	10.064	1.00	15.23
ATOM	742	CG2	ILE	93	-12.417	11.385	9.348	1.00	15.85
ATOM	743	CG1	ILE	93	-13.583	11.170	11.527	1.00	16.63
ATOM	744	CD1	ILE	93	-14.001	10.011	12.392	1.00	19.72
ATOM	745	C	ILE	93	-16.097	11.024	10.300	1.00	12.61
ATOM	746	O	ILE	93	-16.665	9.939	10.458	1.00	11.80
ATOM	747	N	PHE	94	-16.496	12.132	10.916	1.00	13.10
ATOM	748	CA	PHE	94	-17.599	12.070	11.867	1.00	14.24
ATOM	749	CB	PHE	94	-17.266	12.926	13.097	1.00	14.31
ATOM	750	CG	PHE	94	-16.170	12.347	13.960	1.00	12.81
ATOM	751	CD1	PHE	94	-15.026	13.085	14.242	1.00	12.57
ATOM	752	CD2	PHE	94	-16.271	11.052	14.466	1.00	12.32
ATOM	753	CE1	PHE	94	-13.998	12.543	15.007	1.00	11.72
ATOM	754	CE2	PHE	94	-15.254	10.503	15.230	1.00	12.23
ATOM	755	CZ	PHE	94	-14.113	11.243	15.502	1.00	11.57
ATOM	756	C	PHE	94	-18.989	12.420	11.328	1.00	15.81
ATOM	757	O	PHE	94	-19.986	11.862	11.780	1.00	16.53
ATOM	758	N	HIS	95	-19.060	13.326	10.360	1.00	17.45
ATOM	759	CA	HIS	95	-20.348	13.708	9.794	1.00	18.89
ATOM	760	CB	HIS	95	-20.360	15.198	9.436	1.00	21.14
ATOM	761	CG	HIS	95	-20.224	16.104	10.621	1.00	23.42
ATOM	762	CD2	HIS	95	-19.406	17.160	10.848	1.00	23.77
ATOM	763	ND1	HIS	95	-20.999	15.970	11.754	1.00	24.79
ATOM	764	CE1	HIS	95	-20.662	16.902	12.628	1.00	24.61
ATOM	765	NE2	HIS	95	-19.698	17.638	12.102	1.00	24.53
ATOM	766	C	HIS	95	-20.654	12.888	8.558	1.00	19.43
ATOM	767	O	HIS	95	-21.649	12.183	8.504	1.00	19.80
ATOM	768	N	ASN	96	-19.784	12.976	7.565	1.00	18.86
ATOM	769	CA	ASN	96	-19.972	12.265	6.307	1.00	18.38
ATOM	770	CB	ASN	96	-18.944	12.761	5.297	1.00	21.28
ATOM	771	CG	ASN	96	-19.172	14.199	4.914	1.00	23.62
ATOM	772	OD1	ASN	96	-19.810	14.485	3.890	1.00	24.96
ATOM	773	ND2	ASN	96	-18.681	15.126	5.740	1.00	23.92
ATOM	774	C	ASN	96	-19.904	10.753	6.397	1.00	17.65
ATOM	775	O	ASN	96	-20.840	10.067	5.981	1.00	16.43
ATOM	776	N	PHE	97	-18.791	10.232	6.910	1.00	16.52
ATOM	777	CA	PHE	97	-18.617	8.784	7.051	1.00	15.56
ATOM	778	CB	PHE	97	-17.122	8.415	7.163	1.00	15.90
ATOM	779	CG	PHE	97	-16.340	8.601	5.893	1.00	16.94
ATOM	780	CD1	PHE	97	-15.804	9.841	5.563	1.00	17.15
ATOM	781	CD2	PHE	97	-16.124	7.526	5.025	1.00	17.23
ATOM	782	CE1	PHE	97	-15.061	10.011	4.382	1.00	17.56
ATOM	783	CE2	PHE	97	-15.389	7.683	3.849	1.00	16.87
ATOM	784	CZ	PHE	97	-14.857	8.930	3.526	1.00	16.91
ATOM	785	C	PHE	97	-19.362	8.249	8.284	1.00	15.54
ATOM	786	O	PHE	97	-19.558	7.041	8.426	1.00	16.30
ATOM	787	N	ASN	98	-19.752	9.157	9.173	1.00	14.64
ATOM	788	CA	ASN	98	-20.481	8.820	10.404	1.00	14.60
ATOM	789	CB	ASN	98	-21.930	8.442	10.078	1.00	16.90
ATOM	790	CG	ASN	98	-22.788	8.308	11.312	1.00	17.74
ATOM	791	OD1	ASN	98	-23.499	7.306	11.483	1.00	20.80
ATOM	792	ND2	ASN	98	-22.738	9.315	12.186	1.00	19.17

ATOM	793	C	ASN	98	-19.878	7.724	11.284	1.00	13.51
ATOM	794	O	ASN	98	-20.591	6.847	11.776	1.00	13.41
ATOM	795	N	TYR	99	-18.566	7.764	11.490	1.00	12.07
ATOM	796	CA	TYR	99	-17.924	6.789	12.358	1.00	10.77
ATOM	797	CB	TYR	99	-16.442	6.680	12.035	1.00	10.35
ATOM	798	CG	TYR	99	-16.174	5.953	10.745	1.00	11.37
ATOM	799	CD1	TYR	99	-15.623	6.617	9.645	1.00	11.13
ATOM	800	CE1	TYR	99	-15.298	5.929	8.479	1.00	13.85
ATOM	801	CD2	TYR	99	-16.412	4.585	10.645	1.00	12.91
ATOM	802	CE2	TYR	99	-16.096	3.881	9.480	1.00	13.79
ATOM	803	CZ	TYR	99	-15.529	4.560	8.408	1.00	13.16
ATOM	804	OH	TYR	99	-15.124	3.846	7.306	1.00	16.23
ATOM	805	C	TYR	99	-18.122	7.280	13.789	1.00	10.62
ATOM	806	O	TYR	99	-18.310	8.477	14.018	1.00	10.26
ATOM	807	N	PRO	100	-18.080	6.366	14.775	1.00	10.09
ATOM	808	CD	PRO	100	-18.119	4.900	14.637	1.00	10.72
ATOM	809	CA	PRO	100	-18.273	6.753	16.175	1.00	9.90
ATOM	810	CB	PRO	100	-18.884	5.490	16.785	1.00	10.72
ATOM	811	CG	PRO	100	-18.168	4.430	16.087	1.00	11.14
ATOM	812	C	PRO	100	-17.015	7.196	16.915	1.00	9.59
ATOM	813	O	PRO	100	-17.095	7.671	18.039	1.00	10.54
ATOM	814	N	ALA	101	-15.868	7.039	16.267	1.00	10.30
ATOM	815	CA	ALA	101	-14.582	7.410	16.847	1.00	9.12
ATOM	816	CB	ALA	101	-14.242	6.476	18.012	1.00	10.24
ATOM	817	C	ALA	101	-13.538	7.283	15.754	1.00	8.52
ATOM	818	O	ALA	101	-13.836	6.806	14.661	1.00	9.37
ATOM	819	N	ALA	102	-12.313	7.713	16.035	1.00	7.71
ATOM	820	CA	ALA	102	-11.258	7.618	15.041	1.00	7.08
ATOM	821	CB	ALA	102	-11.486	8.648	13.956	1.00	9.03
ATOM	822	C	ALA	102	-9.877	7.808	15.641	1.00	7.24
ATOM	823	O	ALA	102	-9.704	8.549	16.614	1.00	7.33
ATOM	824	N	VAL	103	-8.896	7.133	15.049	1.00	7.22
ATOM	825	CA	VAL	103	-7.509	7.267	15.472	1.00	7.78
ATOM	826	CB	VAL	103	-6.740	5.931	15.430	1.00	8.44
ATOM	827	CG1	VAL	103	-5.247	6.183	15.701	1.00	9.55
ATOM	828	CG2	VAL	103	-7.290	4.970	16.482	1.00	7.66
ATOM	829	C	VAL	103	-6.909	8.200	14.439	1.00	8.27
ATOM	830	O	VAL	103	-6.889	7.885	13.251	1.00	8.35
ATOM	831	N	VAL	104	-6.433	9.348	14.904	1.00	8.83
ATOM	832	CA	VAL	104	-5.841	10.356	14.036	1.00	8.58
ATOM	833	CB	VAL	104	-6.150	11.760	14.567	1.00	7.96
ATOM	834	CG1	VAL	104	-5.595	12.810	13.628	1.00	10.45
ATOM	835	CG2	VAL	104	-7.655	11.911	14.758	1.00	9.47
ATOM	836	C	VAL	104	-4.331	10.193	13.973	1.00	8.73
ATOM	837	O	VAL	104	-3.655	10.064	14.991	1.00	7.99
ATOM	838	N	VAL	105	-3.799	10.186	12.765	1.00	9.15
ATOM	839	CA	VAL	105	-2.369	10.052	12.617	1.00	10.22
ATOM	840	CB	VAL	105	-1.941	8.612	12.361	1.00	11.07
ATOM	841	CG1	VAL	105	-2.414	8.115	10.988	1.00	8.70
ATOM	842	CG2	VAL	105	-.470	8.568	12.465	1.00	13.64
ATOM	843	C	VAL	105	-1.837	10.896	11.482	1.00	11.52
ATOM	844	O	VAL	105	-2.492	11.076	10.462	1.00	12.14
ATOM	845	N	GLU	106	-.638	11.425	11.661	1.00	11.87
ATOM	846	CA	GLU	106	-.049	12.224	10.610	1.00	12.75
ATOM	847	CB	GLU	106	.670	13.409	11.242	1.00	17.67
ATOM	848	CG	GLU	106	-.351	14.407	11.802	1.00	21.65
ATOM	849	CD	GLU	106	.260	15.733	12.169	1.00	24.08
ATOM	850	OE1	GLU	106	1.343	15.710	12.786	1.00	25.43
ATOM	851	OE2	GLU	106	-.346	16.792	11.859	1.00	24.71
ATOM	852	C	GLU	106	.847	11.358	9.714	1.00	12.87

ATOM	853	O	GLU	106	1.305	10.278	10.127	1.00	10.68
ATOM	854	N	ASP	107	1.071	11.821	8.484	1.00	13.26
ATOM	855	CA	ASP	107	1.860	11.089	7.495	1.00	13.98
ATOM	856	CB	ASP	107	1.683	11.743	6.120	1.00	15.37
ATOM	857	CG	ASP	107	2.212	13.160	6.079	1.00	17.19
ATOM	858	OD1	ASP	107	2.295	13.803	7.144	1.00	18.58
ATOM	859	OD2	ASP	107	2.532	13.650	4.976	1.00	18.81
ATOM	860	C	ASP	107	3.356	10.845	7.749	1.00	14.48
ATOM	861	O	ASP	107	4.032	10.256	6.901	1.00	14.30
ATOM	862	N	ASP	108	3.885	11.282	8.888	1.00	13.82
ATOM	863	CA	ASP	108	5.294	11.028	9.182	1.00	13.82
ATOM	864	CB	ASP	108	6.046	12.339	9.459	1.00	16.85
ATOM	865	CG	ASP	108	5.510	13.083	10.662	1.00	17.91
ATOM	866	OD1	ASP	108	4.369	12.802	11.076	1.00	19.13
ATOM	867	OD2	ASP	108	6.227	13.969	11.188	1.00	20.65
ATOM	868	C	ASP	108	5.431	10.079	10.373	1.00	12.85
ATOM	869	O	ASP	108	6.472	10.033	11.024	1.00	11.62
ATOM	870	N	LEU	109	4.382	9.311	10.648	1.00	12.51
ATOM	871	CA	LEU	109	4.429	8.369	11.756	1.00	11.84
ATOM	872	CB	LEU	109	3.205	8.549	12.665	1.00	11.21
ATOM	873	CG	LEU	109	3.070	9.941	13.301	1.00	11.05
ATOM	874	CD1	LEU	109	1.827	10.008	14.221	1.00	10.98
ATOM	875	CD2	LEU	109	4.341	10.248	14.071	1.00	11.00
ATOM	876	C	LEU	109	4.497	6.921	11.283	1.00	11.37
ATOM	877	O	LEU	109	3.889	6.554	10.280	1.00	12.80
ATOM	878	N	GLU	110	5.279	6.117	11.999	1.00	10.93
ATOM	879	CA	GLU	110	5.411	4.691	11.716	1.00	10.60
ATOM	880	CB	GLU	110	6.879	4.284	11.637	1.00	13.25
ATOM	881	CG	GLU	110	7.050	2.783	11.492	1.00	16.53
ATOM	882	CD	GLU	110	8.474	2.380	11.210	1.00	19.05
ATOM	883	OE1	GLU	110	9.144	3.110	10.452	1.00	20.09
ATOM	884	OE2	GLU	110	8.920	1.323	11.719	1.00	21.02
ATOM	885	C	GLU	110	4.760	3.977	12.897	1.00	11.09
ATOM	886	O	GLU	110	4.953	4.392	14.035	1.00	10.92
ATOM	887	N	VAL	111	3.988	2.925	12.639	1.00	9.94
ATOM	888	CA	VAL	111	3.339	2.215	13.745	1.00	10.18
ATOM	889	CB	VAL	111	1.889	1.810	13.400	1.00	9.46
ATOM	890	CG1	VAL	111	1.085	3.027	13.098	1.00	8.93
ATOM	891	CG2	VAL	111	1.870	.843	12.221	1.00	10.73
ATOM	892	C	VAL	111	4.042	.970	14.257	1.00	10.03
ATOM	893	O	VAL	111	4.742	.265	13.517	1.00	10.11
ATOM	894	N	ALA	112	3.833	.700	15.543	1.00	8.80
ATOM	895	CA	ALA	112	4.386	-.478	16.206	1.00	9.08
ATOM	896	CB	ALA	112	4.321	-.295	17.707	1.00	7.44
ATOM	897	C	ALA	112	3.501	-1.653	15.791	1.00	8.11
ATOM	898	O	ALA	112	2.385	-1.447	15.318	1.00	7.79
ATOM	899	N	PRO	113	3.988	-2.895	15.954	1.00	7.96
ATOM	900	CD	PRO	113	5.362	-3.259	16.338	1.00	8.88
ATOM	901	CA	PRO	113	3.221	-4.092	15.589	1.00	7.60
ATOM	902	CB	PRO	113	4.166	-5.231	15.951	1.00	9.08
ATOM	903	CG	PRO	113	5.520	-4.620	15.702	1.00	12.43
ATOM	904	C	PRO	113	1.894	-4.209	16.326	1.00	7.40
ATOM	905	O	PRO	113	.941	-4.764	15.783	1.00	7.92
ATOM	906	N	ASP	114	1.831	-3.692	17.555	1.00	7.43
ATOM	907	CA	ASP	114	.594	-3.777	18.322	1.00	7.47
ATOM	908	CB	ASP	114	.854	-4.298	19.753	1.00	7.24
ATOM	909	CG	ASP	114	1.944	-3.532	20.483	1.00	8.99
ATOM	910	OD1	ASP	114	2.398	-2.469	19.993	1.00	8.51
ATOM	911	OD2	ASP	114	2.342	-4.010	21.564	1.00	8.71
ATOM	912	C	ASP	114	-.207	-2.479	18.360	1.00	6.64

ATOM	913	O	ASP	114	-1.062	-2.289	19.213	1.00	7.12
ATOM	914	N	PHE	115	.048	-1.600	17.400	1.00	6.86
ATOM	915	CA	PHE	115	-.669	-.322	17.287	1.00	7.18
ATOM	916	CB	PHE	115	-.240	.357	15.978	1.00	8.46
ATOM	917	CG	PHE	115	-1.001	1.611	15.649	1.00	7.70
ATOM	918	CD1	PHE	115	-.591	2.845	16.140	1.00	7.70
ATOM	919	CD2	PHE	115	-2.119	1.556	14.820	1.00	8.31
ATOM	920	CE1	PHE	115	-1.289	4.018	15.803	1.00	7.96
ATOM	921	CE2	PHE	115	-2.820	2.718	14.482	1.00	7.90
ATOM	922	CZ	PHE	115	-2.404	3.950	14.973	1.00	7.75
ATOM	923	C	PHE	115	-2.198	-.537	17.293	1.00	7.21
ATOM	924	O	PHE	115	-2.923	.089	18.073	1.00	5.72
ATOM	925	N	PHE	116	-2.676	-1.437	16.431	1.00	7.10
ATOM	926	CA	PHE	116	-4.109	-1.711	16.332	1.00	7.59
ATOM	927	CB	PHE	116	-4.417	-2.524	15.066	1.00	8.55
ATOM	928	CG	PHE	116	-4.004	-1.837	13.795	1.00	9.09
ATOM	929	CD1	PHE	116	-2.723	-2.022	13.268	1.00	8.77
ATOM	930	CD2	PHE	116	-4.877	-.975	13.142	1.00	8.68
ATOM	931	CE1	PHE	116	-2.318	-1.357	12.109	1.00	9.05
ATOM	932	CE2	PHE	116	-4.478	-.308	11.981	1.00	8.56
ATOM	933	CZ	PHE	116	-3.184	-.507	11.468	1.00	7.83
ATOM	934	C	PHE	116	-4.683	-2.422	17.544	1.00	6.42
ATOM	935	O	PHE	116	-5.769	-2.083	18.004	1.00	7.05
ATOM	936	N	GLU	117	-3.951	-3.411	18.051	1.00	7.13
ATOM	937	CA	GLU	117	-4.369	-4.175	19.221	1.00	7.16
ATOM	938	CB	GLU	117	-3.281	-5.205	19.560	1.00	7.12
ATOM	939	CG	GLU	117	-3.476	-6.014	20.851	1.00	8.19
ATOM	940	CD	GLU	117	-4.461	-7.161	20.718	1.00	8.15
ATOM	941	OE1	GLU	117	-4.841	-7.521	19.582	1.00	8.41
ATOM	942	OE2	GLU	117	-4.844	-7.722	21.766	1.00	8.34
ATOM	943	C	GLU	117	-4.549	-3.210	20.380	1.00	7.36
ATOM	944	O	GLU	117	-5.499	-3.320	21.165	1.00	7.62
ATOM	945	N	TYR	118	-3.627	-2.257	20.476	1.00	7.12
ATOM	946	CA	TYR	118	-3.647	-1.257	21.535	1.00	6.20
ATOM	947	CB	TYR	118	-2.401	-.372	21.417	1.00	6.09
ATOM	948	CG	TYR	118	-2.381	.839	22.326	1.00	6.82
ATOM	949	CD1	TYR	118	-2.322	.705	23.710	1.00	6.78
ATOM	950	CE1	TYR	118	-2.255	1.827	24.547	1.00	6.87
ATOM	951	CD2	TYR	118	-2.382	2.129	21.790	1.00	6.70
ATOM	952	CE2	TYR	118	-2.317	3.257	22.609	1.00	6.45
ATOM	953	CZ	TYR	118	-2.247	3.098	23.990	1.00	7.18
ATOM	954	OH	TYR	118	-2.130	4.201	24.807	1.00	6.73
ATOM	955	C	TYR	118	-4.918	-.403	21.504	1.00	6.05
ATOM	956	O	TYR	118	-5.615	-.261	22.517	1.00	7.30
ATOM	957	N	PHE	119	-5.244	.158	20.349	1.00	5.77
ATOM	958	CA	PHE	119	-6.447	.971	20.291	1.00	6.35
ATOM	959	CB	PHE	119	-6.440	1.839	19.031	1.00	6.94
ATOM	960	CG	PHE	119	-5.499	3.006	19.131	1.00	6.40
ATOM	961	CD1	PHE	119	-4.338	3.066	18.357	1.00	7.15
ATOM	962	CD2	PHE	119	-5.748	4.029	20.048	1.00	5.79
ATOM	963	CE1	PHE	119	-3.433	4.135	18.501	1.00	7.96
ATOM	964	CE2	PHE	119	-4.867	5.090	20.202	1.00	8.25
ATOM	965	CZ	PHE	119	-3.699	5.148	19.428	1.00	8.15
ATOM	966	C	PHE	119	-7.732	.168	20.426	1.00	5.91
ATOM	967	O	PHE	119	-8.720	.676	20.948	1.00	7.33
ATOM	968	N	GLN	120	-7.723	-1.087	19.993	1.00	7.70
ATOM	969	CA	GLN	120	-8.918	-1.915	20.123	1.00	7.76
ATOM	970	CB	GLN	120	-8.731	-3.252	19.390	1.00	10.72
ATOM	971	CG	GLN	120	-9.978	-4.145	19.324	1.00	14.25
ATOM	972	CD	GLN	120	-11.071	-3.605	18.385	1.00	16.03

ATOM	973	OE1	GLN	120	-10.851	-3.439	17.177	1.00	19.47
ATOM	974	NE2	GLN	120	-12.244	-3.347	18.934	1.00	17.37
ATOM	975	C	GLN	120	-9.172	-2.169	21.616	1.00	7.68
ATOM	976	O	GLN	120	-10.310	-2.125	22.088	1.00	7.65
ATOM	977	N	ALA	121	-8.097	-2.424	22.350	1.00	7.79
ATOM	978	CA	ALA	121	-8.183	-2.709	23.778	1.00	7.97
ATOM	979	CB	ALA	121	-6.857	-3.276	24.260	1.00	7.86
ATOM	980	C	ALA	121	-8.569	-1.510	24.637	1.00	8.37
ATOM	981	O	ALA	121	-9.296	-1.661	25.613	1.00	8.18
ATOM	982	N	THR	122	-8.086	-.323	24.275	1.00	7.55
ATOM	983	CA	THR	122	-8.357	.901	25.034	1.00	8.16
ATOM	984	CB	THR	122	-7.152	1.854	24.955	1.00	8.44
ATOM	985	OG1	THR	122	-6.837	2.116	23.584	1.00	6.66
ATOM	986	CG2	THR	122	-5.937	1.223	25.637	1.00	7.80
ATOM	987	C	THR	122	-9.622	1.686	24.659	1.00	8.29
ATOM	988	O	THR	122	-10.103	2.506	25.449	1.00	7.74
ATOM	989	N	TYR	123	-10.160	1.447	23.467	1.00	8.16
ATOM	990	CA	TYR	123	-11.379	2.123	23.034	1.00	8.82
ATOM	991	CB	TYR	123	-11.789	1.601	21.649	1.00	9.68
ATOM	992	CG	TYR	123	-13.094	2.133	21.088	1.00	10.25
ATOM	993	CD1	TYR	123	-13.459	3.475	21.222	1.00	10.80
ATOM	994	CE1	TYR	123	-14.641	3.964	20.637	1.00	11.45
ATOM	995	CD2	TYR	123	-13.936	1.299	20.366	1.00	12.08
ATOM	996	CE2	TYR	123	-15.109	1.769	19.783	1.00	12.18
ATOM	997	CZ	TYR	123	-15.455	3.105	19.920	1.00	11.72
ATOM	998	OH	TYR	123	-16.612	3.568	19.319	1.00	14.14
ATOM	999	C	TYR	123	-12.498	1.923	24.079	1.00	9.40
ATOM	1000	O	TYR	123	-13.206	2.873	24.429	1.00	8.84
ATOM	1001	N	PRO	124	-12.653	.695	24.614	1.00	9.63
ATOM	1002	CD	PRO	124	-11.958	-.562	24.296	1.00	10.50
ATOM	1003	CA	PRO	124	-13.713	.491	25.616	1.00	10.22
ATOM	1004	CB	PRO	124	-13.596	-1.004	25.963	1.00	10.46
ATOM	1005	CG	PRO	124	-12.965	-1.611	24.709	1.00	12.41
ATOM	1006	C	PRO	124	-13.549	1.390	26.848	1.00	9.99
ATOM	1007	O	PRO	124	-14.544	1.888	27.398	1.00	9.95
ATOM	1008	N	LEU	125	-12.306	1.591	27.291	1.00	10.04
ATOM	1009	CA	LEU	125	-12.045	2.447	28.451	1.00	11.38
ATOM	1010	CB	LEU	125	-10.550	2.439	28.825	1.00	14.34
ATOM	1011	CG	LEU	125	-9.997	1.309	29.701	1.00	17.36
ATOM	1012	CD1	LEU	125	-10.453	1.464	31.163	1.00	17.76
ATOM	1013	CD2	LEU	125	-10.447	-.021	29.133	1.00	17.74
ATOM	1014	C	LEU	125	-12.468	3.878	28.156	1.00	10.59
ATOM	1015	O	LEU	125	-13.065	4.545	28.998	1.00	10.50
ATOM	1016	N	LEU	126	-12.121	4.355	26.964	1.00	10.79
ATOM	1017	CA	LEU	126	-12.457	5.709	26.556	1.00	9.59
ATOM	1018	CB	LEU	126	-11.869	5.999	25.171	1.00	8.74
ATOM	1019	CG	LEU	126	-12.098	7.408	24.615	1.00	9.34
ATOM	1020	CD1	LEU	126	-11.528	8.475	25.574	1.00	9.40
ATOM	1021	CD2	LEU	126	-11.457	7.494	23.225	1.00	10.36
ATOM	1022	C	LEU	126	-13.962	5.898	26.519	1.00	10.19
ATOM	1023	O	LEU	126	-14.476	6.927	26.940	1.00	10.25
ATOM	1024	N	LYS	127	-14.675	4.909	25.995	1.00	11.87
ATOM	1025	CA	LYS	127	-16.125	5.008	25.939	1.00	12.96
ATOM	1026	CB	LYS	127	-16.710	3.829	25.155	1.00	14.46
ATOM	1027	CG	LYS	127	-16.569	3.908	23.640	1.00	15.57
ATOM	1028	CD	LYS	127	-17.129	2.639	22.964	1.00	18.67
ATOM	1029	CE	LYS	127	-18.418	2.172	23.654	1.00	21.11
ATOM	1030	NZ	LYS	127	-18.958	.818	23.244	1.00	23.89
ATOM	1031	C	LYS	127	-16.735	5.031	27.340	1.00	12.65
ATOM	1032	O	LYS	127	-17.669	5.789	27.597	1.00	13.41

ATOM	1033	N	ALA	128	-16.196	4.226	28.250	1.00	13.56
ATOM	1034	CA	ALA	128	-16.749	4.145	29.596	1.00	13.17
ATOM	1035	CB	ALA	128	-16.419	2.781	30.205	1.00	14.59
ATOM	1036	C	ALA	128	-16.372	5.261	30.572	1.00	14.85
ATOM	1037	O	ALA	128	-17.229	5.744	31.330	1.00	15.68
ATOM	1038	N	ASP	129	-15.119	5.703	30.528	1.00	11.59
ATOM	1039	CA	ASP	129	-14.633	6.716	31.467	1.00	11.87
ATOM	1040	CB	ASP	129	-13.188	6.388	31.864	1.00	12.86
ATOM	1041	CG	ASP	129	-12.728	7.166	33.083	1.00	12.19
ATOM	1042	OD1	ASP	129	-13.468	8.075	33.517	1.00	12.60
ATOM	1043	OD2	ASP	129	-11.616	6.887	33.600	1.00	14.15
ATOM	1044	C	ASP	129	-14.706	8.149	30.937	1.00	11.50
ATOM	1045	O	ASP	129	-13.856	8.573	30.160	1.00	10.92
ATOM	1046	N	PRO	130	-15.698	8.933	31.394	1.00	10.68
ATOM	1047	CD	PRO	130	-16.757	8.602	32.367	1.00	11.02
ATOM	1048	CA	PRO	130	-15.829	10.314	30.920	1.00	10.51
ATOM	1049	CB	PRO	130	-17.199	10.733	31.460	1.00	11.96
ATOM	1050	CG	PRO	130	-17.298	9.969	32.746	1.00	11.87
ATOM	1051	C	PRO	130	-14.695	11.241	31.359	1.00	10.27
ATOM	1052	O	PRO	130	-14.587	12.386	30.879	1.00	10.02
ATOM	1053	N	SER	131	-13.853	10.758	32.272	1.00	9.76
ATOM	1054	CA	SER	131	-12.722	11.560	32.732	1.00	9.06
ATOM	1055	CB	SER	131	-12.269	11.144	34.137	1.00	8.67
ATOM	1056	OG	SER	131	-11.696	9.849	34.183	1.00	9.58
ATOM	1057	C	SER	131	-11.566	11.441	31.741	1.00	8.36
ATOM	1058	O	SER	131	-10.536	12.097	31.887	1.00	9.25
ATOM	1059	N	LEU	132	-11.743	10.582	30.742	1.00	7.83
ATOM	1060	CA	LEU	132	-10.753	10.405	29.684	1.00	7.34
ATOM	1061	CB	LEU	132	-10.586	8.927	29.330	1.00	7.83
ATOM	1062	CG	LEU	132	-9.835	8.043	30.307	1.00	7.63
ATOM	1063	CD1	LEU	132	-9.892	6.585	29.802	1.00	8.16
ATOM	1064	CD2	LEU	132	-8.383	8.532	30.433	1.00	8.62
ATOM	1065	C	LEU	132	-11.312	11.100	28.458	1.00	7.18
ATOM	1066	O	LEU	132	-12.532	11.091	28.241	1.00	8.54
ATOM	1067	N	TRP	133	-10.441	11.714	27.662	1.00	7.31
ATOM	1068	CA	TRP	133	-10.906	12.320	26.430	1.00	6.12
ATOM	1069	CB	TRP	133	-10.968	13.859	26.558	1.00	6.94
ATOM	1070	CG	TRP	133	-9.697	14.660	26.413	1.00	8.34
ATOM	1071	CD2	TRP	133	-9.596	16.000	25.900	1.00	8.06
ATOM	1072	CE2	TRP	133	-8.242	16.389	26.005	1.00	8.76
ATOM	1073	CE3	TRP	133	-10.522	16.911	25.362	1.00	9.42
ATOM	1074	CD1	TRP	133	-8.435	14.303	26.797	1.00	9.67
ATOM	1075	NE1	TRP	133	-7.558	15.336	26.555	1.00	9.17
ATOM	1076	CZ2	TRP	133	-7.784	17.654	25.588	1.00	9.54
ATOM	1077	CZ3	TRP	133	-10.063	18.170	24.944	1.00	9.18
ATOM	1078	CH2	TRP	133	-8.709	18.521	25.061	1.00	9.20
ATOM	1079	C	TRP	133	-10.089	11.841	25.228	1.00	7.29
ATOM	1080	O	TRP	133	-10.376	12.204	24.089	1.00	7.06
ATOM	1081	N	CYS	134	-9.109	10.977	25.487	1.00	5.85
ATOM	1082	CA	CYS	134	-8.280	10.401	24.420	1.00	7.12
ATOM	1083	C	CYS	134	-7.386	9.236	24.824	1.00	7.24
ATOM	1084	O	CYS	134	-7.178	8.950	26.009	1.00	5.62
ATOM	1085	CB	CYS	134	-7.413	11.500	23.775	1.00	8.81
ATOM	1086	SG	CYS	134	-5.588	11.482	23.996	1.00	10.88
ATOM	1087	N	VAL	135	-6.904	8.526	23.808	1.00	7.59
ATOM	1088	CA	VAL	135	-5.940	7.448	24.003	1.00	6.99
ATOM	1089	CB	VAL	135	-6.478	6.049	23.631	1.00	7.33
ATOM	1090	CG1	VAL	135	-5.339	5.030	23.711	1.00	8.00
ATOM	1091	CG2	VAL	135	-7.615	5.648	24.572	1.00	7.51
ATOM	1092	C	VAL	135	-4.842	7.818	23.017	1.00	7.32

ATOM	1093	O	VAL	135	-5.112	8.061	21.838	1.00	6.25
ATOM	1094	N	SER	136	-3.606	7.892	23.503	1.00	6.26
ATOM	1095	CA	SER	136	-2.493	8.238	22.632	1.00	6.28
ATOM	1096	CB	SER	136	-1.829	9.547	23.084	1.00	7.02
ATOM	1097	OG	SER	136	-.660	9.810	22.319	1.00	8.26
ATOM	1098	C	SER	136	-1.465	7.126	22.623	1.00	6.43
ATOM	1099	O	SER	136	-1.287	6.414	23.611	1.00	5.52
ATOM	1100	N	ALA	137	-.799	6.979	21.489	1.00	5.39
ATOM	1101	CA	ALA	137	.236	5.976	21.341	1.00	6.40
ATOM	1102	CB	ALA	137	.322	5.529	19.883	1.00	6.08
ATOM	1103	C	ALA	137	1.578	6.559	21.763	1.00	5.50
ATOM	1104	O	ALA	137	2.575	5.860	21.758	1.00	6.01
ATOM	1105	N	TRP	138	1.595	7.824	22.173	1.00	5.82
ATOM	1106	CA	TRP	138	2.859	8.499	22.487	1.00	6.38
ATOM	1107	CB	TRP	138	2.855	9.844	21.756	1.00	6.96
ATOM	1108	CG	TRP	138	4.189	10.536	21.661	1.00	8.21
ATOM	1109	CD2	TRP	138	5.150	10.404	20.602	1.00	9.11
ATOM	1110	CE2	TRP	138	6.230	11.256	20.911	1.00	9.84
ATOM	1111	CE3	TRP	138	5.199	9.646	19.419	1.00	9.52
ATOM	1112	CD1	TRP	138	4.716	11.439	22.547	1.00	9.05
ATOM	1113	NE1	TRP	138	5.942	11.880	22.099	1.00	9.42
ATOM	1114	CZ2	TRP	138	7.358	11.376	20.079	1.00	9.82
ATOM	1115	CZ3	TRP	138	6.327	9.767	18.585	1.00	10.61
ATOM	1116	CH2	TRP	138	7.390	10.631	18.930	1.00	10.27
ATOM	1117	C	TRP	138	3.294	8.730	23.930	1.00	6.83
ATOM	1118	O	TRP	138	2.522	9.217	24.761	1.00	6.27
ATOM	1119	N	ASN	139	4.552	8.383	24.211	1.00	7.68
ATOM	1120	CA	ASN	139	5.151	8.632	25.526	1.00	7.51
ATOM	1121	CB	ASN	139	5.935	7.417	26.039	1.00	7.42
ATOM	1122	CG	ASN	139	6.681	7.703	27.350	1.00	8.64
ATOM	1123	OD1	ASN	139	6.721	8.838	27.838	1.00	7.27
ATOM	1124	ND2	ASN	139	7.284	6.676	27.911	1.00	8.18
ATOM	1125	C	ASN	139	6.121	9.793	25.290	1.00	8.00
ATOM	1126	O	ASN	139	7.170	9.619	24.659	1.00	6.82
ATOM	1127	N	ASP	140	5.770	10.973	25.793	1.00	7.69
ATOM	1128	CA	ASP	140	6.614	12.148	25.616	1.00	8.76
ATOM	1129	CB	ASP	140	5.916	13.357	26.241	1.00	11.53
ATOM	1130	CG	ASP	140	4.903	13.998	25.283	1.00	13.95
ATOM	1131	OD1	ASP	140	5.327	14.633	24.287	1.00	17.07
ATOM	1132	OD2	ASP	140	3.681	13.858	25.508	1.00	17.20
ATOM	1133	C	ASP	140	8.070	11.978	26.114	1.00	9.09
ATOM	1134	O	ASP	140	8.998	12.593	25.572	1.00	9.65
ATOM	1135	N	ASN	141	8.291	11.128	27.113	1.00	10.21
ATOM	1136	CA	ASN	141	9.660	10.870	27.576	1.00	10.07
ATOM	1137	CB	ASN	141	9.780	11.062	29.085	1.00	10.94
ATOM	1138	CG	ASN	141	9.682	12.509	29.488	1.00	10.87
ATOM	1139	OD1	ASN	141	10.469	13.341	29.040	1.00	11.83
ATOM	1140	ND2	ASN	141	8.720	12.820	30.337	1.00	10.96
ATOM	1141	C	ASN	141	9.982	9.424	27.233	1.00	10.71
ATOM	1142	O	ASN	141	10.519	8.686	28.053	1.00	11.22
ATOM	1143	N	GLY	142	9.677	9.035	26.000	1.00	9.00
ATOM	1144	CA	GLY	142	9.883	7.660	25.600	1.00	8.94
ATOM	1145	C	GLY	142	11.183	7.244	24.958	1.00	9.31
ATOM	1146	O	GLY	142	11.186	6.290	24.187	1.00	7.86
ATOM	1147	N	LYS	143	12.285	7.930	25.239	1.00	10.59
ATOM	1148	CA	LYS	143	13.539	7.482	24.642	1.00	12.11
ATOM	1149	CB	LYS	143	14.646	8.523	24.803	1.00	15.92
ATOM	1150	CG	LYS	143	15.053	8.792	26.231	1.00	20.50
ATOM	1151	CD	LYS	143	16.178	9.821	26.263	1.00	23.30
ATOM	1152	CE	LYS	143	15.698	11.223	25.885	1.00	25.10

ATOM	1153	NZ	LYS	143	16.846	12.184	25.755	1.00	27.36
ATOM	1154	C	LYS	143	13.950	6.158	25.288	1.00	11.71
ATOM	1155	O	LYS	143	13.541	5.832	26.407	1.00	10.38
ATOM	1156	N	GLU	144	14.741	5.394	24.549	1.00	12.36
ATOM	1157	CA	GLU	144	15.248	4.090	24.949	1.00	13.93
ATOM	1158	CB	GLU	144	16.445	3.759	24.046	1.00	19.98
ATOM	1159	CG	GLU	144	17.211	2.493	24.390	1.00	25.95
ATOM	1160	CD	GLU	144	16.526	1.241	23.880	1.00	28.71
ATOM	1161	OE1	GLU	144	16.408	1.082	22.638	1.00	30.76
ATOM	1162	OE2	GLU	144	16.105	.410	24.710	1.00	30.64
ATOM	1163	C	GLU	144	15.669	3.938	26.413	1.00	13.51
ATOM	1164	O	GLU	144	15.227	3.023	27.116	1.00	12.43
ATOM	1165	N	GLN	145	16.532	4.834	26.864	1.00	13.24
ATOM	1166	CA	GLN	145	17.047	4.768	28.220	1.00	13.31
ATOM	1167	CB	GLN	145	18.324	5.608	28.326	1.00	16.15
ATOM	1168	CG	GLN	145	19.477	5.129	27.439	1.00	20.52
ATOM	1169	CD	GLN	145	19.864	3.671	27.673	1.00	22.46
ATOM	1170	OE1	GLN	145	20.175	3.251	28.806	1.00	24.19
ATOM	1171	NE2	GLN	145	19.863	2.884	26.601	1.00	24.21
ATOM	1172	C	GLN	145	16.066	5.202	29.292	1.00	11.92
ATOM	1173	O	GLN	145	16.356	5.086	30.475	1.00	11.38
ATOM	1174	N	MET	146	14.898	5.695	28.896	1.00	10.76
ATOM	1175	CA	MET	146	13.949	6.160	29.887	1.00	10.75
ATOM	1176	CB	MET	146	13.631	7.637	29.630	1.00	13.76
ATOM	1177	CG	MET	146	14.879	8.523	29.770	1.00	17.41
ATOM	1178	SD	MET	146	14.554	10.213	29.396	1.00	23.24
ATOM	1179	CE	MET	146	13.325	10.605	30.645	1.00	20.85
ATOM	1180	C	MET	146	12.672	5.347	29.976	1.00	10.13
ATOM	1181	O	MET	146	11.731	5.752	30.647	1.00	9.47
ATOM	1182	N	VAL	147	12.655	4.200	29.307	1.00	8.91
ATOM	1183	CA	VAL	147	11.497	3.313	29.335	1.00	8.75
ATOM	1184	CB	VAL	147	10.790	3.225	27.966	1.00	9.02
ATOM	1185	CG1	VAL	147	10.373	4.587	27.526	1.00	9.18
ATOM	1186	CG2	VAL	147	11.706	2.565	26.925	1.00	12.10
ATOM	1187	C	VAL	147	11.945	1.910	29.742	1.00	9.36
ATOM	1188	O	VAL	147	13.092	1.517	29.483	1.00	9.63
ATOM	1189	N	ASP	148	11.048	1.178	30.397	1.00	9.33
ATOM	1190	CA	ASP	148	11.323	-.181	30.849	1.00	9.46
ATOM	1191	CB	ASP	148	10.572	-.479	32.155	1.00	10.96
ATOM	1192	CG	ASP	148	10.930	-1.840	32.739	1.00	11.39
ATOM	1193	OD1	ASP	148	11.672	-2.610	32.078	1.00	12.01
ATOM	1194	OD2	ASP	148	10.464	-2.146	33.859	1.00	12.71
ATOM	1195	C	ASP	148	10.915	-1.181	29.772	1.00	9.32
ATOM	1196	O	ASP	148	9.723	-1.481	29.593	1.00	8.98
ATOM	1197	N	SER	149	11.915	-1.706	29.066	1.00	9.72
ATOM	1198	CA	SER	149	11.678	-2.657	27.987	1.00	10.33
ATOM	1199	CB	SER	149	12.973	-2.898	27.202	1.00	12.23
ATOM	1200	OG	SER	149	13.262	-1.793	26.366	1.00	17.97
ATOM	1201	C	SER	149	11.107	-3.980	28.447	1.00	9.06
ATOM	1202	O	SER	149	10.668	-4.792	27.623	1.00	9.48
ATOM	1203	N	SER	150	11.120	-4.210	29.758	1.00	9.33
ATOM	1204	CA	SER	150	10.566	-5.448	30.298	1.00	8.88
ATOM	1205	CB	SER	150	11.280	-5.855	31.599	1.00	10.05
ATOM	1206	OG	SER	150	10.914	-5.033	32.699	1.00	11.44
ATOM	1207	C	SER	150	9.074	-5.262	30.578	1.00	8.80
ATOM	1208	O	SER	150	8.390	-6.210	30.941	1.00	9.36
ATOM	1209	N	LYS	151	8.575	-4.038	30.404	1.00	7.08
ATOM	1210	CA	LYS	151	7.160	-3.748	30.662	1.00	7.09
ATOM	1211	CB	LYS	151	7.024	-2.839	31.894	1.00	7.95
ATOM	1212	CG	LYS	151	7.372	-3.516	33.217	1.00	7.53

ATOM	1213	CD	LYS	151	6.376	-4.618	33.580	1.00	9.01
ATOM	1214	CE	LYS	151	4.968	-4.083	33.874	1.00	9.63
ATOM	1215	NZ	LYS	151	4.034	-5.217	34.218	1.00	7.97
ATOM	1216	C	LYS	151	6.463	-3.096	29.463	1.00	6.52
ATOM	1217	O	LYS	151	5.867	-2.020	29.576	1.00	7.14
ATOM	1218	N	PRO	152	6.536	-3.736	28.285	1.00	7.11
ATOM	1219	CD	PRO	152	7.141	-5.047	27.982	1.00	6.63
ATOM	1220	CA	PRO	152	5.890	-3.169	27.099	1.00	7.22
ATOM	1221	CB	PRO	152	6.296	-4.141	25.989	1.00	7.76
ATOM	1222	CG	PRO	152	6.401	-5.446	26.712	1.00	8.45
ATOM	1223	C	PRO	152	4.371	-3.050	27.240	1.00	6.77
ATOM	1224	O	PRO	152	3.726	-2.327	26.480	1.00	6.69
ATOM	1225	N	GLU	153	3.802	-3.746	28.219	1.00	7.00
ATOM	1226	CA	GLU	153	2.350	-3.708	28.417	1.00	7.39
ATOM	1227	CB	GLU	153	1.875	-5.077	28.946	1.00	8.59
ATOM	1228	CG	GLU	153	2.164	-5.353	30.429	1.00	9.32
ATOM	1229	CD	GLU	153	3.550	-5.950	30.719	1.00	10.33
ATOM	1230	OE1	GLU	153	4.515	-5.714	29.958	1.00	9.93
ATOM	1231	OE2	GLU	153	3.671	-6.666	31.745	1.00	11.62
ATOM	1232	C	GLU	153	1.876	-2.581	29.364	1.00	7.26
ATOM	1233	O	GLU	153	.700	-2.234	29.397	1.00	7.48
ATOM	1234	N	LEU	154	2.797	-2.003	30.125	1.00	7.27
ATOM	1235	CA	LEU	154	2.440	-.955	31.090	1.00	6.87
ATOM	1236	CB	LEU	154	3.670	-.608	31.931	1.00	7.29
ATOM	1237	CG	LEU	154	3.376	.301	33.125	1.00	7.21
ATOM	1238	CD1	LEU	154	2.284	-.319	33.975	1.00	9.49
ATOM	1239	CD2	LEU	154	4.625	.479	33.944	1.00	9.02
ATOM	1240	C	LEU	154	1.841	.337	30.504	1.00	6.51
ATOM	1241	O	LEU	154	2.437	.953	29.629	1.00	6.54
ATOM	1242	N	LEU	155	.666	.742	30.995	1.00	6.00
ATOM	1243	CA	LEU	155	.023	1.969	30.509	1.00	6.53
ATOM	1244	CB	LEU	155	-1.331	1.661	29.869	1.00	5.74
ATOM	1245	CG	LEU	155	-1.340	.619	28.755	1.00	5.84
ATOM	1246	CD1	LEU	155	-2.779	.454	28.254	1.00	7.35
ATOM	1247	CD2	LEU	155	-.421	1.040	27.629	1.00	6.94
ATOM	1248	C	LEU	155	-.193	2.960	31.653	1.00	6.64
ATOM	1249	O	LEU	155	-.156	2.576	32.824	1.00	7.45
ATOM	1250	N	TYR	156	-.445	4.223	31.302	1.00	5.79
ATOM	1251	CA	TYR	156	-.636	5.299	32.288	1.00	6.00
ATOM	1252	CB	TYR	156	.624	6.184	32.395	1.00	6.25
ATOM	1253	CG	TYR	156	1.914	5.516	32.802	1.00	7.06
ATOM	1254	CD1	TYR	156	2.683	4.802	31.882	1.00	6.99
ATOM	1255	CE1	TYR	156	3.893	4.217	32.260	1.00	6.83
ATOM	1256	CD2	TYR	156	2.379	5.627	34.109	1.00	7.87
ATOM	1257	CE2	TYR	156	3.578	5.048	34.502	1.00	7.60
ATOM	1258	CZ	TYR	156	4.333	4.345	33.571	1.00	8.20
ATOM	1259	OH	TYR	156	5.531	3.792	33.950	1.00	8.79
ATOM	1260	C	TYR	156	-1.744	6.255	31.873	1.00	5.60
ATOM	1261	O	TYR	156	-2.264	6.184	30.764	1.00	6.19
ATOM	1262	N	ARG	157	-2.104	7.149	32.789	1.00	6.67
ATOM	1263	CA	ARG	157	-3.043	8.210	32.469	1.00	7.18
ATOM	1264	CB	ARG	157	-4.114	8.398	33.563	1.00	7.14
ATOM	1265	CG	ARG	157	-5.134	7.268	33.660	1.00	8.40
ATOM	1266	CD	ARG	157	-6.105	7.499	34.837	1.00	9.57
ATOM	1267	NE	ARG	157	-6.985	8.655	34.664	1.00	12.10
ATOM	1268	CZ	ARG	157	-8.255	8.587	34.259	1.00	10.96
ATOM	1269	NH1	ARG	157	-8.818	7.416	33.980	1.00	11.57
ATOM	1270	NH2	ARG	157	-8.965	9.699	34.130	1.00	11.83
ATOM	1271	C	ARG	157	-2.117	9.436	32.429	1.00	6.66
ATOM	1272	O	ARG	157	-1.085	9.467	33.123	1.00	7.91

ATOM	1273	N	THR	158	-2.458	10.415	31.591	1.00	6.03
ATOM	1274	CA	THR	158	-1.683	11.658	31.471	1.00	5.98
ATOM	1275	CB	THR	158	-.649	11.612	30.306	1.00	6.79
ATOM	1276	OG1	THR	158	.060	12.860	30.246	1.00	7.64
ATOM	1277	CG2	THR	158	-1.341	11.371	28.981	1.00	7.38
ATOM	1278	C	THR	158	-2.610	12.846	31.230	1.00	6.74
ATOM	1279	O	THR	158	-3.618	12.730	30.534	1.00	5.50
ATOM	1280	N	ASP	159	-2.262	13.982	31.827	1.00	6.00
ATOM	1281	CA	ASP	159	-3.040	15.209	31.688	1.00	7.56
ATOM	1282	CB	ASP	159	-2.875	16.094	32.927	1.00	7.23
ATOM	1283	CG	ASP	159	-3.643	15.577	34.114	1.00	8.29
ATOM	1284	OD1	ASP	159	-3.131	15.686	35.250	1.00	8.22
ATOM	1285	OD2	ASP	159	-4.763	15.068	33.907	1.00	10.35
ATOM	1286	C	ASP	159	-2.566	15.993	30.483	1.00	7.91
ATOM	1287	O	ASP	159	-3.244	16.924	30.039	1.00	8.96
ATOM	1288	N	PHE	160	-1.395	15.622	29.973	1.00	7.60
ATOM	1289	CA	PHE	160	-.810	16.286	28.818	1.00	8.66
ATOM	1290	CB	PHE	160	.727	16.283	28.944	1.00	7.74
ATOM	1291	CG	PHE	160	1.420	17.166	27.949	1.00	8.49
ATOM	1292	CD1	PHE	160	1.757	18.479	28.282	1.00	10.20
ATOM	1293	CD2	PHE	160	1.693	16.707	26.656	1.00	9.21
ATOM	1294	CE1	PHE	160	2.355	19.326	27.345	1.00	10.11
ATOM	1295	CE2	PHE	160	2.293	17.557	25.706	1.00	8.33
ATOM	1296	CZ	PHE	160	2.623	18.866	26.053	1.00	10.56
ATOM	1297	C	PHE	160	-1.230	15.552	27.540	1.00	8.78
ATOM	1298	O	PHE	160	-.798	14.422	27.296	1.00	9.90
ATOM	1299	N	PHE	161	-2.086	16.188	26.741	1.00	8.87
ATOM	1300	CA	PHE	161	-2.545	15.615	25.471	1.00	8.40
ATOM	1301	CB	PHE	161	-3.582	16.540	24.818	1.00	8.16
ATOM	1302	CG	PHE	161	-3.901	16.184	23.393	1.00	9.46
ATOM	1303	CD1	PHE	161	-4.460	14.946	23.071	1.00	9.45
ATOM	1304	CD2	PHE	161	-3.628	17.087	22.365	1.00	9.68
ATOM	1305	CE1	PHE	161	-4.741	14.614	21.737	1.00	10.15
ATOM	1306	CE2	PHE	161	-3.904	16.769	21.036	1.00	9.08
ATOM	1307	CZ	PHE	161	-4.459	15.534	20.715	1.00	9.85
ATOM	1308	C	PHE	161	-1.322	15.466	24.570	1.00	8.36
ATOM	1309	O	PHE	161	-.738	16.452	24.134	1.00	9.12
ATOM	1310	N	PRO	162	-.936	14.224	24.256	1.00	8.42
ATOM	1311	CD	PRO	162	-1.405	12.951	24.827	1.00	8.67
ATOM	1312	CA	PRO	162	.242	13.999	23.412	1.00	9.67
ATOM	1313	CB	PRO	162	.694	12.585	23.798	1.00	9.79
ATOM	1314	CG	PRO	162	-.097	12.238	25.037	1.00	9.42
ATOM	1315	C	PRO	162	.070	14.088	21.909	1.00	10.19
ATOM	1316	O	PRO	162	1.027	14.397	21.210	1.00	11.04
ATOM	1317	N	GLY	163	-1.130	13.809	21.411	1.00	10.03
ATOM	1318	CA	GLY	163	-1.331	13.793	19.968	1.00	10.47
ATOM	1319	C	GLY	163	-.496	12.619	19.470	1.00	10.70
ATOM	1320	O	GLY	163	-.391	11.593	20.168	1.00	10.38
ATOM	1321	N	LEU	164	.098	12.757	18.285	1.00	9.58
ATOM	1322	CA	LEU	164	.984	11.738	17.709	1.00	9.25
ATOM	1323	CB	LEU	164	2.336	11.797	18.427	1.00	10.98
ATOM	1324	CG	LEU	164	3.027	13.144	18.215	1.00	11.11
ATOM	1325	CD1	LEU	164	4.137	13.329	19.220	1.00	12.02
ATOM	1326	CD2	LEU	164	3.539	13.231	16.802	1.00	12.79
ATOM	1327	C	LEU	164	.421	10.324	17.748	1.00	8.14
ATOM	1328	O	LEU	164	1.044	9.401	18.265	1.00	7.73
ATOM	1329	N	GLY	165	-.759	10.171	17.161	1.00	6.99
ATOM	1330	CA	GLY	165	-1.432	8.888	17.145	1.00	7.52
ATOM	1331	C	GLY	165	-2.408	8.870	18.304	1.00	6.65
ATOM	1332	O	GLY	165	-2.094	8.373	19.381	1.00	8.02

ATOM	1333	N	TRP	166	-3.597	9.415	18.085	1.00	6.41
ATOM	1334	CA	TRP	166	-4.566	9.477	19.157	1.00	6.32
ATOM	1335	CB	TRP	166	-4.523	10.860	19.799	1.00	7.09
ATOM	1336	CG	TRP	166	-4.734	12.006	18.840	1.00	7.90
ATOM	1337	CD2	TRP	166	-5.873	12.877	18.786	1.00	8.47
ATOM	1338	CE2	TRP	166	-5.623	13.837	17.776	1.00	8.09
ATOM	1339	CE3	TRP	166	-7.078	12.938	19.497	1.00	9.00
ATOM	1340	CD1	TRP	166	-3.865	12.457	17.882	1.00	7.24
ATOM	1341	NE1	TRP	166	-4.391	13.561	17.241	1.00	8.05
ATOM	1342	CZ2	TRP	166	-6.537	14.847	17.462	1.00	9.85
ATOM	1343	CZ3	TRP	166	-7.988	13.944	19.184	1.00	10.40
ATOM	1344	CH2	TRP	166	-7.710	14.885	18.177	1.00	7.94
ATOM	1345	C	TRP	166	-5.986	9.178	18.718	1.00	7.01
ATOM	1346	O	TRP	166	-6.416	9.555	17.628	1.00	6.87
ATOM	1347	N	LEU	167	-6.707	8.519	19.618	1.00	6.42
ATOM	1348	CA	LEU	167	-8.095	8.123	19.431	1.00	6.73
ATOM	1349	CB	LEU	167	-8.281	6.724	20.021	1.00	8.16
ATOM	1350	CG	LEU	167	-9.699	6.198	20.205	1.00	7.93
ATOM	1351	CD1	LEU	167	-10.301	5.872	18.847	1.00	9.31
ATOM	1352	CD2	LEU	167	-9.635	4.942	21.087	1.00	8.44
ATOM	1353	C	LEU	167	-9.034	9.094	20.153	1.00	7.02
ATOM	1354	O	LEU	167	-8.790	9.449	21.299	1.00	6.10
ATOM	1355	N	LEU	168	-10.085	9.540	19.469	1.00	7.10
ATOM	1356	CA	LEU	168	-11.078	10.413	20.092	1.00	7.44
ATOM	1357	CB	LEU	168	-10.936	11.884	19.642	1.00	6.68
ATOM	1358	CG	LEU	168	-11.480	12.319	18.267	1.00	7.19
ATOM	1359	CD1	LEU	168	-11.768	13.828	18.260	1.00	8.22
ATOM	1360	CD2	LEU	168	-10.482	11.954	17.173	1.00	6.02
ATOM	1361	C	LEU	168	-12.451	9.894	19.682	1.00	7.86
ATOM	1362	O	LEU	168	-12.578	9.163	18.699	1.00	7.31
ATOM	1363	N	LEU	169	-13.473	10.279	20.438	1.00	8.32
ATOM	1364	CA	LEU	169	-14.844	9.880	20.155	1.00	8.62
ATOM	1365	CB	LEU	169	-15.626	9.670	21.460	1.00	8.21
ATOM	1366	CG	LEU	169	-15.051	8.708	22.496	1.00	9.55
ATOM	1367	CD1	LEU	169	-15.984	8.613	23.697	1.00	9.19
ATOM	1368	CD2	LEU	169	-14.870	7.362	21.858	1.00	9.39
ATOM	1369	C	LEU	169	-15.546	10.984	19.366	1.00	8.31
ATOM	1370	O	LEU	169	-15.184	12.157	19.453	1.00	8.32
ATOM	1371	N	ALA	170	-16.563	10.590	18.609	1.00	8.37
ATOM	1372	CA	ALA	170	-17.356	11.532	17.837	1.00	9.63
ATOM	1373	CB	ALA	170	-18.441	10.783	17.078	1.00	9.68
ATOM	1374	C	ALA	170	-17.984	12.559	18.785	1.00	10.16
ATOM	1375	O	ALA	170	-18.179	13.726	18.425	1.00	9.14
ATOM	1376	N	GLU	171	-18.294	12.132	20.003	1.00	10.57
ATOM	1377	CA	GLU	171	-18.896	13.058	20.965	1.00	12.45
ATOM	1378	CB	GLU	171	-19.330	12.311	22.221	1.00	16.20
ATOM	1379	CG	GLU	171	-20.414	11.295	21.940	1.00	21.08
ATOM	1380	CD	GLU	171	-20.422	10.195	22.967	1.00	23.82
ATOM	1381	OE1	GLU	171	-20.703	10.505	24.143	1.00	26.36
ATOM	1382	OE2	GLU	171	-20.138	9.029	22.609	1.00	25.67
ATOM	1383	C	GLU	171	-17.946	14.191	21.311	1.00	12.15
ATOM	1384	O	GLU	171	-18.389	15.328	21.512	1.00	10.82
ATOM	1385	N	LEU	172	-16.645	13.899	21.360	1.00	10.58
ATOM	1386	CA	LEU	172	-15.677	14.947	21.648	1.00	10.38
ATOM	1387	CB	LEU	172	-14.288	14.367	21.905	1.00	10.07
ATOM	1388	CG	LEU	172	-13.201	15.443	22.070	1.00	10.71
ATOM	1389	CD1	LEU	172	-13.579	16.375	23.224	1.00	11.65
ATOM	1390	CD2	LEU	172	-11.833	14.813	22.307	1.00	10.05
ATOM	1391	C	LEU	172	-15.626	15.895	20.458	1.00	10.10
ATOM	1392	O	LEU	172	-15.513	17.104	20.621	1.00	10.05

ATOM	1393	N	TRP	173	-15.687	15.346	19.250	1.00	10.65
ATOM	1394	CA	TRP	173	-15.685	16.216	18.087	1.00	11.40
ATOM	1395	CB	TRP	173	-15.713	15.402	16.794	1.00	13.02
ATOM	1396	CG	TRP	173	-15.715	16.266	15.580	1.00	15.56
ATOM	1397	CD2	TRP	173	-14.731	17.253	15.215	1.00	16.48
ATOM	1398	CE2	TRP	173	-15.179	17.862	14.019	1.00	17.30
ATOM	1399	CE3	TRP	173	-13.519	17.680	15.784	1.00	18.08
ATOM	1400	CD1	TRP	173	-16.679	16.316	14.616	1.00	16.43
ATOM	1401	NE1	TRP	173	-16.364	17.271	13.676	1.00	16.39
ATOM	1402	CZ2	TRP	173	-14.457	18.885	13.377	1.00	17.87
ATOM	1403	CZ3	TRP	173	-12.797	18.705	15.139	1.00	18.60
ATOM	1404	CH2	TRP	173	-13.277	19.291	13.948	1.00	18.67
ATOM	1405	C	TRP	173	-16.912	17.138	18.159	1.00	10.84
ATOM	1406	O	TRP	173	-16.849	18.293	17.756	1.00	11.32
ATOM	1407	N	ALA	174	-18.028	16.637	18.684	1.00	11.29
ATOM	1408	CA	ALA	174	-19.245	17.456	18.783	1.00	11.12
ATOM	1409	CB	ALA	174	-20.390	16.634	19.369	1.00	12.86
ATOM	1410	C	ALA	174	-18.986	18.673	19.661	1.00	11.21
ATOM	1411	O	ALA	174	-19.495	19.773	19.413	1.00	11.67
ATOM	1412	N	GLU	175	-18.185	18.458	20.692	1.00	11.15
ATOM	1413	CA	GLU	175	-17.817	19.489	21.652	1.00	11.54
ATOM	1414	CB	GLU	175	-17.265	18.815	22.906	1.00	12.20
ATOM	1415	CG	GLU	175	-16.740	19.763	23.948	1.00	12.43
ATOM	1416	CD	GLU	175	-16.173	19.035	25.152	1.00	11.75
ATOM	1417	OE1	GLU	175	-16.346	17.801	25.250	1.00	13.30
ATOM	1418	OE2	GLU	175	-15.557	19.700	26.006	1.00	14.40
ATOM	1419	C	GLU	175	-16.783	20.491	21.134	1.00	11.15
ATOM	1420	O	GLU	175	-16.874	21.687	21.419	1.00	10.20
ATOM	1421	N	LEU	176	-15.804	19.999	20.376	1.00	10.76
ATOM	1422	CA	LEU	176	-14.725	20.836	19.846	1.00	11.06
ATOM	1423	CB	LEU	176	-13.455	19.991	19.660	1.00	10.91
ATOM	1424	CG	LEU	176	-12.898	19.323	20.921	1.00	10.67
ATOM	1425	CD1	LEU	176	-11.633	18.524	20.597	1.00	10.73
ATOM	1426	CD2	LEU	176	-12.585	20.391	21.932	1.00	11.69
ATOM	1427	C	LEU	176	-14.985	21.594	18.538	1.00	11.48
ATOM	1428	O	LEU	176	-14.475	22.702	18.356	1.00	12.23
ATOM	1429	N	GLU	177	-15.756	20.997	17.635	1.00	13.31
ATOM	1430	CA	GLU	177	-16.014	21.604	16.330	1.00	13.94
ATOM	1431	CB	GLU	177	-16.958	20.716	15.507	1.00	16.19
ATOM	1432	CG	GLU	177	-16.960	21.048	14.019	1.00	19.24
ATOM	1433	CD	GLU	177	-17.771	20.058	13.208	1.00	21.44
ATOM	1434	OE1	GLU	177	-17.306	19.656	12.101	1.00	23.89
ATOM	1435	OE2	GLU	177	-18.875	19.675	13.665	1.00	22.23
ATOM	1436	C	GLU	177	-16.540	23.038	16.351	1.00	14.11
ATOM	1437	O	GLU	177	-16.029	23.887	15.620	1.00	14.87
ATOM	1438	N	PRO	178	-17.565	23.330	17.182	1.00	14.13
ATOM	1439	CD	PRO	178	-18.344	22.382	18.002	1.00	14.50
ATOM	1440	CA	PRO	178	-18.135	24.686	17.264	1.00	14.20
ATOM	1441	CB	PRO	178	-19.200	24.561	18.351	1.00	14.41
ATOM	1442	CG	PRO	178	-19.639	23.149	18.255	1.00	15.27
ATOM	1443	C	PRO	178	-17.146	25.802	17.606	1.00	13.88
ATOM	1444	O	PRO	178	-17.375	26.966	17.272	1.00	15.45
ATOM	1445	N	LYS	179	-16.054	25.462	18.279	1.00	11.92
ATOM	1446	CA	LYS	179	-15.085	26.474	18.680	1.00	10.96
ATOM	1447	CB	LYS	179	-15.066	26.570	20.211	1.00	10.39
ATOM	1448	CG	LYS	179	-14.850	25.214	20.897	1.00	10.59
ATOM	1449	CD	LYS	179	-14.688	25.353	22.408	1.00	10.92
ATOM	1450	CE	LYS	179	-14.375	24.023	23.073	1.00	12.06
ATOM	1451	NZ	LYS	179	-14.115	24.160	24.545	1.00	12.27
ATOM	1452	C	LYS	179	-13.683	26.200	18.150	1.00	10.79

ATOM	1453	O	LYS	179	-12.705	26.777	18.635	1.00	10.66
ATOM	1454	N	TRP	180	-13.587	25.316	17.162	1.00	9.87
ATOM	1455	CA	TRP	180	-12.292	24.973	16.574	1.00	10.73
ATOM	1456	CB	TRP	180	-12.497	24.121	15.328	1.00	11.27
ATOM	1457	CG	TRP	180	-11.244	23.456	14.867	1.00	12.04
ATOM	1458	CD2	TRP	180	-10.585	22.349	15.491	1.00	12.62
ATOM	1459	CE2	TRP	180	-9.433	22.065	14.723	1.00	13.08
ATOM	1460	CE3	TRP	180	-10.853	21.571	16.625	1.00	13.45
ATOM	1461	CD1	TRP	180	-10.487	23.789	13.779	1.00	13.58
ATOM	1462	NE1	TRP	180	-9.405	22.959	13.689	1.00	12.65
ATOM	1463	CZ2	TRP	180	-8.543	21.030	15.054	1.00	13.26
ATOM	1464	CZ3	TRP	180	-9.968	20.538	16.960	1.00	13.95
ATOM	1465	CH2	TRP	180	-8.827	20.281	16.173	1.00	14.20
ATOM	1466	C	TRP	180	-11.494	26.240	16.244	1.00	10.27
ATOM	1467	O	TRP	180	-12.010	27.167	15.628	1.00	11.59
ATOM	1468	N	PRO	181	-10.198	26.266	16.616	1.00	11.08
ATOM	1469	CD	PRO	181	-9.442	25.152	17.234	1.00	9.96
ATOM	1470	CA	PRO	181	-9.325	27.423	16.386	1.00	11.73
ATOM	1471	CB	PRO	181	-8.179	27.178	17.366	1.00	10.96
ATOM	1472	CG	PRO	181	-8.005	25.686	17.262	1.00	10.85
ATOM	1473	C	PRO	181	-8.814	27.698	14.982	1.00	12.32
ATOM	1474	O	PRO	181	-8.807	26.829	14.101	1.00	12.80
ATOM	1475	N	LYS	182	-8.361	28.931	14.797	1.00	13.24
ATOM	1476	CA	LYS	182	-7.817	29.367	13.527	1.00	13.29
ATOM	1477	CB	LYS	182	-7.677	30.890	13.515	1.00	16.40
ATOM	1478	CG	LYS	182	-8.978	31.665	13.401	1.00	19.81
ATOM	1479	CD	LYS	182	-9.399	31.889	11.946	1.00	23.66
ATOM	1480	CE	LYS	182	-9.777	30.584	11.225	1.00	25.30
ATOM	1481	NZ	LYS	182	-11.083	29.986	11.661	1.00	28.01
ATOM	1482	C	LYS	182	-6.447	28.729	13.282	1.00	13.06
ATOM	1483	O	LYS	182	-6.078	28.476	12.133	1.00	11.41
ATOM	1484	N	ALA	183	-5.703	28.482	14.362	1.00	12.13
ATOM	1485	CA	ALA	183	-4.377	27.873	14.265	1.00	12.46
ATOM	1486	CB	ALA	183	-3.371	28.887	13.734	1.00	12.52
ATOM	1487	C	ALA	183	-3.892	27.316	15.605	1.00	12.71
ATOM	1488	O	ALA	183	-4.504	27.557	16.652	1.00	12.70
ATOM	1489	N	PHE	184	-2.801	26.558	15.550	1.00	11.62
ATOM	1490	CA	PHE	184	-2.200	25.964	16.737	1.00	11.67
ATOM	1491	CB	PHE	184	-1.623	27.083	17.611	1.00	12.44
ATOM	1492	CG	PHE	184	-.635	27.948	16.880	1.00	14.03
ATOM	1493	CD1	PHE	184	-.920	29.285	16.617	1.00	14.18
ATOM	1494	CD2	PHE	184	.554	27.406	16.406	1.00	14.83
ATOM	1495	CE1	PHE	184	-.038	30.075	15.888	1.00	15.57
ATOM	1496	CE2	PHE	184	1.452	28.184	15.673	1.00	15.69
ATOM	1497	CZ	PHE	184	1.153	29.523	15.414	1.00	15.10
ATOM	1498	C	PHE	184	-3.247	25.147	17.492	1.00	11.45
ATOM	1499	O	PHE	184	-3.441	25.314	18.687	1.00	11.62
ATOM	1500	N	TRP	185	-3.906	24.254	16.762	1.00	9.96
ATOM	1501	CA	TRP	185	-4.969	23.418	17.309	1.00	10.20
ATOM	1502	CB	TRP	185	-5.566	22.540	16.205	1.00	9.69
ATOM	1503	CG	TRP	185	-4.665	21.421	15.784	1.00	9.40
ATOM	1504	CD2	TRP	185	-4.593	20.101	16.359	1.00	8.83
ATOM	1505	CE2	TRP	185	-3.561	19.409	15.689	1.00	9.07
ATOM	1506	CE3	TRP	185	-5.301	19.443	17.374	1.00	8.69
ATOM	1507	CD1	TRP	185	-3.706	21.467	14.818	1.00	10.29
ATOM	1508	NE1	TRP	185	-3.037	20.263	14.753	1.00	10.24
ATOM	1509	CZ2	TRP	185	-3.211	18.083	16.002	1.00	10.34
ATOM	1510	CZ3	TRP	185	-4.956	18.128	17.688	1.00	9.84
ATOM	1511	CH2	TRP	185	-3.917	17.462	17.003	1.00	9.23
ATOM	1512	C	TRP	185	-4.605	22.522	18.488	1.00	9.23

ATOM	1513	O	TRP	185	-5.421	22.348	19.402	1.00	9.10
ATOM	1514	N	ASP	186	-3.396	21.962	18.488	1.00	9.68
ATOM	1515	CA	ASP	186	-3.036	21.073	19.576	1.00	10.00
ATOM	1516	CB	ASP	186	-1.914	20.100	19.159	1.00	11.60
ATOM	1517	CG	ASP	186	-.702	20.783	18.553	1.00	13.90
ATOM	1518	OD1	ASP	186	.358	20.133	18.570	1.00	15.51
ATOM	1519	OD2	ASP	186	-.789	21.930	18.061	1.00	15.89
ATOM	1520	C	ASP	186	-2.729	21.790	20.894	1.00	9.29
ATOM	1521	O	ASP	186	-3.113	21.302	21.944	1.00	10.14
ATOM	1522	N	ASP	187	-2.074	22.945	20.858	1.00	10.11
ATOM	1523	CA	ASP	187	-1.832	23.650	22.114	1.00	9.76
ATOM	1524	CB	ASP	187	-.813	24.783	21.931	1.00	10.68
ATOM	1525	CG	ASP	187	.620	24.278	21.862	1.00	12.20
ATOM	1526	OD1	ASP	187	.898	23.151	22.338	1.00	11.79
ATOM	1527	OD2	ASP	187	1.473	25.025	21.350	1.00	14.36
ATOM	1528	C	ASP	187	-3.182	24.214	22.585	1.00	9.34
ATOM	1529	O	ASP	187	-3.408	24.424	23.779	1.00	8.48
ATOM	1530	N	TRP	188	-4.076	24.461	21.629	1.00	9.05
ATOM	1531	CA	TRP	188	-5.404	24.956	21.945	1.00	8.44
ATOM	1532	CB	TRP	188	-6.135	25.302	20.642	1.00	9.30
ATOM	1533	CG	TRP	188	-7.582	25.633	20.803	1.00	10.43
ATOM	1534	CD2	TRP	188	-8.682	24.741	20.619	1.00	10.32
ATOM	1535	CE2	TRP	188	-9.862	25.481	20.850	1.00	10.05
ATOM	1536	CE3	TRP	188	-8.786	23.384	20.280	1.00	10.45
ATOM	1537	CD1	TRP	188	-8.121	26.847	21.132	1.00	10.38
ATOM	1538	NE1	TRP	188	-9.488	26.765	21.161	1.00	12.05
ATOM	1539	CZ2	TRP	188	-11.134	24.914	20.753	1.00	11.15
ATOM	1540	CZ3	TRP	188	-10.053	22.816	20.179	1.00	10.35
ATOM	1541	CH2	TRP	188	-11.211	23.582	20.417	1.00	10.49
ATOM	1542	C	TRP	188	-6.149	23.850	22.714	1.00	9.05
ATOM	1543	O	TRP	188	-6.872	24.110	23.681	1.00	7.95
ATOM	1544	N	MET	189	-5.959	22.603	22.305	1.00	7.86
ATOM	1545	CA	MET	189	-6.650	21.539	23.022	1.00	8.09
ATOM	1546	CB	MET	189	-6.572	20.220	22.256	1.00	9.93
ATOM	1547	CG	MET	189	-7.732	20.018	21.270	1.00	12.22
ATOM	1548	SD	MET	189	-7.464	18.543	20.329	1.00	14.01
ATOM	1549	CE	MET	189	-7.974	17.292	21.557	1.00	12.28
ATOM	1550	C	MET	189	-6.070	21.357	24.413	1.00	8.12
ATOM	1551	O	MET	189	-6.742	20.845	25.303	1.00	9.14
ATOM	1552	N	ARG	190	-4.821	21.775	24.589	1.00	8.42
ATOM	1553	CA	ARG	190	-4.135	21.643	25.868	1.00	7.53
ATOM	1554	CB	ARG	190	-2.619	21.675	25.640	1.00	6.24
ATOM	1555	CG	ARG	190	-2.145	20.419	24.922	1.00	9.19
ATOM	1556	CD	ARG	190	-.710	20.492	24.461	1.00	9.84
ATOM	1557	NE	ARG	190	-.346	19.262	23.758	1.00	11.66
ATOM	1558	CZ	ARG	190	.332	19.226	22.617	1.00	13.03
ATOM	1559	NH1	ARG	190	.732	20.355	22.034	1.00	13.99
ATOM	1560	NH2	ARG	190	.605	18.060	22.047	1.00	14.30
ATOM	1561	C	ARG	190	-4.542	22.666	26.912	1.00	8.37
ATOM	1562	O	ARG	190	-4.243	22.503	28.096	1.00	8.44
ATOM	1563	N	ARG	191	-5.231	23.710	26.469	1.00	9.18
ATOM	1564	CA	ARG	191	-5.708	24.756	27.371	1.00	9.17
ATOM	1565	CB	ARG	191	-6.239	25.946	26.563	1.00	8.74
ATOM	1566	CG	ARG	191	-5.181	26.678	25.727	1.00	10.51
ATOM	1567	CD	ARG	191	-5.850	27.705	24.817	1.00	12.10
ATOM	1568	NE	ARG	191	-4.891	28.486	24.041	1.00	12.93
ATOM	1569	CZ	ARG	191	-5.234	29.443	23.177	1.00	14.76
ATOM	1570	NH1	ARG	191	-6.521	29.740	22.977	1.00	15.93
ATOM	1571	NH2	ARG	191	-4.292	30.105	22.511	1.00	14.72
ATOM	1572	C	ARG	191	-6.829	24.182	28.235	1.00	9.31

ATOM	1573	O	ARG	191	-7.585	23.308	27.801	1.00	9.41
ATOM	1574	N	PRO	192	-6.958	24.670	29.480	1.00	9.53
ATOM	1575	CD	PRO	192	-6.155	25.704	30.155	1.00	10.44
ATOM	1576	CA	PRO	192	-8.015	24.153	30.365	1.00	10.01
ATOM	1577	CB	PRO	192	-7.756	24.891	31.680	1.00	10.60
ATOM	1578	CG	PRO	192	-7.098	26.175	31.239	1.00	10.57
ATOM	1579	C	PRO	192	-9.437	24.347	29.837	1.00	10.11
ATOM	1580	O	PRO	192	-10.317	23.519	30.092	1.00	10.23
ATOM	1581	N	GLU	193	-9.656	25.426	29.088	1.00	11.08
ATOM	1582	CA	GLU	193	-10.977	25.705	28.523	1.00	12.07
ATOM	1583	CB	GLU	193	-10.959	27.005	27.709	1.00	13.60
ATOM	1584	CG	GLU	193	-10.629	28.271	28.490	1.00	17.38
ATOM	1585	CD	GLU	193	-9.185	28.336	28.943	1.00	18.36
ATOM	1586	OE1	GLU	193	-8.333	27.681	28.315	1.00	17.34
ATOM	1587	OE2	GLU	193	-8.889	29.061	29.928	1.00	20.41
ATOM	1588	C	GLU	193	-11.440	24.567	27.608	1.00	10.95
ATOM	1589	O	GLU	193	-12.638	24.385	27.394	1.00	12.38
ATOM	1590	N	GLN	194	-10.488	23.826	27.049	1.00	9.76
ATOM	1591	CA	GLN	194	-10.819	22.702	26.178	1.00	9.14
ATOM	1592	CB	GLN	194	-9.922	22.689	24.939	1.00	8.96
ATOM	1593	CG	GLN	194	-10.380	23.584	23.786	1.00	10.32
ATOM	1594	CD	GLN	194	-10.451	25.041	24.177	1.00	12.17
ATOM	1595	OE1	GLN	194	-11.537	25.592	24.390	1.00	11.19
ATOM	1596	NE2	GLN	194	-9.286	25.676	24.289	1.00	11.45
ATOM	1597	C	GLN	194	-10.701	21.355	26.893	1.00	9.51
ATOM	1598	O	GLN	194	-11.608	20.524	26.837	1.00	8.91
ATOM	1599	N	ARG	195	-9.594	21.155	27.597	1.00	8.57
ATOM	1600	CA	ARG	195	-9.350	19.892	28.290	1.00	8.00
ATOM	1601	CB	ARG	195	-7.907	19.869	28.805	1.00	8.34
ATOM	1602	CG	ARG	195	-7.467	18.500	29.319	1.00	8.24
ATOM	1603	CD	ARG	195	-5.975	18.475	29.624	1.00	9.83
ATOM	1604	NE	ARG	195	-5.640	19.147	30.876	1.00	10.39
ATOM	1605	CZ	ARG	195	-5.713	18.567	32.066	1.00	11.15
ATOM	1606	NH1	ARG	195	-6.112	17.306	32.158	1.00	10.88
ATOM	1607	NH2	ARG	195	-5.376	19.236	33.164	1.00	12.18
ATOM	1608	C	ARG	195	-10.330	19.585	29.432	1.00	8.34
ATOM	1609	O	ARG	195	-10.713	18.433	29.629	1.00	7.39
ATOM	1610	N	LYS	196	-10.716	20.616	30.178	1.00	8.63
ATOM	1611	CA	LYS	196	-11.645	20.473	31.294	1.00	9.69
ATOM	1612	CB	LYS	196	-13.079	20.277	30.773	1.00	10.01
ATOM	1613	CG	LYS	196	-13.625	21.453	29.951	1.00	11.09
ATOM	1614	CD	LYS	196	-14.939	21.084	29.266	1.00	13.10
ATOM	1615	CE	LYS	196	-15.463	22.238	28.393	1.00	14.26
ATOM	1616	NZ	LYS	196	-16.675	21.863	27.591	1.00	16.36
ATOM	1617	C	LYS	196	-11.250	19.331	32.244	1.00	9.81
ATOM	1618	O	LYS	196	-12.084	18.505	32.643	1.00	10.62
ATOM	1619	N	GLY	197	-9.963	19.307	32.592	1.00	9.61
ATOM	1620	CA	GLY	197	-9.426	18.311	33.512	1.00	9.67
ATOM	1621	C	GLY	197	-9.376	16.877	33.011	1.00	8.82
ATOM	1622	O	GLY	197	-9.040	15.964	33.766	1.00	8.89
ATOM	1623	N	ARG	198	-9.690	16.654	31.742	1.00	8.64
ATOM	1624	CA	ARG	198	-9.689	15.288	31.229	1.00	8.44
ATOM	1625	CB	ARG	198	-10.629	15.185	30.039	1.00	8.78
ATOM	1626	CG	ARG	198	-12.094	15.267	30.479	1.00	7.32
ATOM	1627	CD	ARG	198	-13.033	15.434	29.320	1.00	8.84
ATOM	1628	NE	ARG	198	-12.817	16.698	28.626	1.00	7.98
ATOM	1629	CZ	ARG	198	-13.641	17.199	27.706	1.00	9.65
ATOM	1630	NH1	ARG	198	-14.740	16.538	27.363	1.00	8.67
ATOM	1631	NH2	ARG	198	-13.373	18.376	27.149	1.00	9.36
ATOM	1632	C	ARG	198	-8.312	14.753	30.879	1.00	8.55

ATOM	1633	O	ARG	198	-7.410	15.502	30.517	1.00	9.32
ATOM	1634	N	ALA	199	-8.167	13.439	30.979	1.00	7.60
ATOM	1635	CA	ALA	199	-6.891	12.785	30.722	1.00	8.39
ATOM	1636	CB	ALA	199	-6.485	11.994	31.952	1.00	8.86
ATOM	1637	C	ALA	199	-6.906	11.860	29.516	1.00	7.44
ATOM	1638	O	ALA	199	-7.942	11.587	28.927	1.00	5.79
ATOM	1639	N	CYS	200	-5.727	11.396	29.140	1.00	8.02
ATOM	1640	CA	CYS	200	-5.610	10.460	28.034	1.00	8.39
ATOM	1641	C	CYS	200	-4.849	9.266	28.570	1.00	7.64
ATOM	1642	O	CYS	200	-4.181	9.352	29.590	1.00	7.98
ATOM	1643	CB	CYS	200	-4.742	10.991	26.908	1.00	9.90
ATOM	1644	SG	CYS	200	-5.295	12.347	25.835	1.00	10.82
ATOM	1645	N	VAL	201	-4.926	8.157	27.856	1.00	7.83
ATOM	1646	CA	VAL	201	-4.163	6.981	28.243	1.00	6.95
ATOM	1647	CB	VAL	201	-4.944	5.681	27.949	1.00	7.02
ATOM	1648	CG1	VAL	201	-4.023	4.477	28.032	1.00	8.68
ATOM	1649	CG2	VAL	201	-6.086	5.521	28.958	1.00	8.76
ATOM	1650	C	VAL	201	-2.908	7.040	27.367	1.00	7.29
ATOM	1651	O	VAL	201	-2.992	7.409	26.200	1.00	7.49
ATOM	1652	N	ARG	202	-1.749	6.724	27.937	1.00	7.15
ATOM	1653	CA	ARG	202	-.512	6.720	27.162	1.00	6.14
ATOM	1654	CB	ARG	202	.249	8.052	27.313	1.00	6.92
ATOM	1655	CG	ARG	202	.823	8.357	28.694	1.00	6.25
ATOM	1656	CD	ARG	202	2.174	7.695	28.897	1.00	8.23
ATOM	1657	NE	ARG	202	2.824	8.114	30.141	1.00	7.47
ATOM	1658	CZ	ARG	202	4.006	7.651	30.550	1.00	9.32
ATOM	1659	NH1	ARG	202	4.657	6.756	29.816	1.00	8.95
ATOM	1660	NH2	ARG	202	4.542	8.080	31.686	1.00	9.30
ATOM	1661	C	ARG	202	.304	5.522	27.626	1.00	6.79
ATOM	1662	O	ARG	202	.136	5.035	28.759	1.00	4.84
ATOM	1663	N	PRO	203	1.198	5.018	26.764	1.00	5.69
ATOM	1664	CD	PRO	203	1.362	5.340	25.332	1.00	5.84
ATOM	1665	CA	PRO	203	2.014	3.853	27.122	1.00	5.44
ATOM	1666	CB	PRO	203	2.099	3.106	25.805	1.00	4.87
ATOM	1667	CG	PRO	203	2.351	4.262	24.857	1.00	6.91
ATOM	1668	C	PRO	203	3.401	4.124	27.665	1.00	6.44
ATOM	1669	O	PRO	203	3.930	5.221	27.547	1.00	7.24
ATOM	1670	N	GLU	204	3.979	3.084	28.251	1.00	6.62
ATOM	1671	CA	GLU	204	5.338	3.133	28.765	1.00	6.33
ATOM	1672	CB	GLU	204	5.631	1.854	29.553	1.00	6.87
ATOM	1673	CG	GLU	204	7.098	1.634	29.945	1.00	8.23
ATOM	1674	CD	GLU	204	7.579	2.549	31.061	1.00	9.93
ATOM	1675	OE1	GLU	204	6.762	3.309	31.633	1.00	11.07
ATOM	1676	OE2	GLU	204	8.788	2.496	31.374	1.00	9.84
ATOM	1677	C	GLU	204	6.252	3.211	27.536	1.00	6.71
ATOM	1678	O	GLU	204	7.244	3.935	27.529	1.00	6.72
ATOM	1679	N	ILE	205	5.895	2.451	26.501	1.00	6.17
ATOM	1680	CA	ILE	205	6.671	2.415	25.261	1.00	6.50
ATOM	1681	CB	ILE	205	7.217	.998	25.010	1.00	5.66
ATOM	1682	CG2	ILE	205	8.137	1.008	23.792	1.00	8.20
ATOM	1683	CG1	ILE	205	7.937	.517	26.274	1.00	8.05
ATOM	1684	CD1	ILE	205	8.654	-.831	26.154	1.00	9.15
ATOM	1685	C	ILE	205	5.750	2.850	24.123	1.00	6.08
ATOM	1686	O	ILE	205	4.682	2.261	23.911	1.00	7.05
ATOM	1687	N	SER	206	6.159	3.898	23.405	1.00	6.75
ATOM	1688	CA	SER	206	5.348	4.446	22.323	1.00	6.49
ATOM	1689	CB	SER	206	6.054	5.647	21.682	1.00	5.79
ATOM	1690	OG	SER	206	6.264	6.672	22.643	1.00	9.05
ATOM	1691	C	SER	206	4.959	3.453	21.239	1.00	6.85
ATOM	1692	O	SER	206	5.722	2.547	20.902	1.00	6.95

ATOM	1693	N	ARG	207	3.758	3.647	20.693	1.00	6.28
ATOM	1694	CA	ARG	207	3.248	2.788	19.631	1.00	6.56
ATOM	1695	CB	ARG	207	1.810	2.342	19.924	1.00	6.07
ATOM	1696	CG	ARG	207	1.741	.901	20.443	1.00	5.70
ATOM	1697	CD	ARG	207	2.558	.725	21.731	1.00	7.08
ATOM	1698	NE	ARG	207	2.643	-.671	22.142	1.00	6.85
ATOM	1699	CZ	ARG	207	3.008	-1.069	23.356	1.00	7.61
ATOM	1700	NH1	ARG	207	3.316	-.177	24.281	1.00	8.79
ATOM	1701	NH2	ARG	207	3.068	-2.358	23.646	1.00	7.47
ATOM	1702	C	ARG	207	3.340	3.454	18.272	1.00	7.00
ATOM	1703	O	ARG	207	2.844	2.925	17.281	1.00	7.40
ATOM	1704	N	THR	208	3.955	4.634	18.255	1.00	7.45
ATOM	1705	CA	THR	208	4.206	5.379	17.022	1.00	9.15
ATOM	1706	CB	THR	208	3.173	6.525	16.769	1.00	9.38
ATOM	1707	OG1	THR	208	3.037	7.319	17.953	1.00	8.53
ATOM	1708	CG2	THR	208	1.815	5.965	16.359	1.00	9.45
ATOM	1709	C	THR	208	5.585	6.020	17.159	1.00	9.69
ATOM	1710	O	THR	208	6.088	6.190	18.268	1.00	8.32
ATOM	1711	N	MET	209	6.200	6.361	16.028	1.00	11.14
ATOM	1712	CA	MET	209	7.500	7.040	16.013	1.00	12.28
ATOM	1713	CB	MET	209	8.679	6.050	15.918	1.00	15.40
ATOM	1714	CG	MET	209	8.865	5.365	14.557	1.00	19.59
ATOM	1715	SD	MET	209	10.474	4.534	14.270	1.00	25.86
ATOM	1716	CE	MET	209	11.542	5.725	14.894	1.00	25.19
ATOM	1717	C	MET	209	7.511	7.950	14.788	1.00	12.20
ATOM	1718	O	MET	209	6.915	7.611	13.769	1.00	10.86
ATOM	1719	N	THR	210	8.166	9.106	14.889	1.00	13.31
ATOM	1720	CA	THR	210	8.234	10.029	13.760	1.00	14.45
ATOM	1721	CB	THR	210	8.392	11.502	14.208	1.00	16.04
ATOM	1722	OG1	THR	210	9.673	11.671	14.830	1.00	16.89
ATOM	1723	CG2	THR	210	7.296	11.900	15.172	1.00	16.31
ATOM	1724	C	THR	210	9.440	9.675	12.903	1.00	15.70
ATOM	1725	O	THR	210	10.419	9.109	13.399	1.00	16.69
ATOM	1726	N	PHE	211	9.362	9.991	11.612	1.00	16.25
ATOM	1727	CA	PHE	211	10.452	9.714	10.676	1.00	16.87
ATOM	1728	CB	PHE	211	10.219	8.381	9.944	1.00	17.21
ATOM	1729	CG	PHE	211	8.981	8.348	9.083	1.00	17.39
ATOM	1730	CD1	PHE	211	8.916	9.073	7.888	1.00	16.70
ATOM	1731	CD2	PHE	211	7.894	7.558	9.444	1.00	17.34
ATOM	1732	CE1	PHE	211	7.804	9.010	7.076	1.00	16.74
ATOM	1733	CE2	PHE	211	6.765	7.494	8.624	1.00	17.04
ATOM	1734	CZ	PHE	211	6.726	8.223	7.441	1.00	17.56
ATOM	1735	C	PHE	211	10.566	10.860	9.673	1.00	17.35
ATOM	1736	O	PHE	211	9.667	11.703	9.607	1.00	18.29
ATOM	1737	N	HIS	225	13.365	16.821	20.203	1.00	33.83
ATOM	1738	CA	HIS	225	13.865	15.453	20.110	1.00	33.72
ATOM	1739	CB	HIS	225	14.804	15.139	21.301	1.00	39.17
ATOM	1740	CG	HIS	225	14.228	15.443	22.652	1.00	43.28
ATOM	1741	CD2	HIS	225	14.201	16.592	23.370	1.00	44.82
ATOM	1742	ND1	HIS	225	13.627	14.484	23.445	1.00	44.96
ATOM	1743	CE1	HIS	225	13.256	15.029	24.590	1.00	45.64
ATOM	1744	NE2	HIS	225	13.593	16.307	24.569	1.00	45.61
ATOM	1745	C	HIS	225	12.788	14.362	19.968	1.00	31.70
ATOM	1746	O	HIS	225	12.868	13.298	20.604	1.00	29.85
ATOM	1747	N	LEU	226	11.789	14.620	19.123	1.00	27.56
ATOM	1748	CA	LEU	226	10.737	13.630	18.882	1.00	24.61
ATOM	1749	CB	LEU	226	9.695	14.151	17.896	1.00	24.35
ATOM	1750	CG	LEU	226	8.680	15.157	18.418	1.00	23.94
ATOM	1751	CD1	LEU	226	7.776	15.586	17.275	1.00	23.42
ATOM	1752	CD2	LEU	226	7.890	14.554	19.576	1.00	22.85

ATOM	1753	C	LEU	226	11.350	12.381	18.276	1.00	23.24
ATOM	1754	O	LEU	226	10.902	11.266	18.531	1.00	21.75
ATOM	1755	N	LYS	227	12.374	12.588	17.451	1.00	21.99
ATOM	1756	CA	LYS	227	13.070	11.509	16.757	1.00	20.84
ATOM	1757	CB	LYS	227	14.150	12.091	15.819	1.00	23.51
ATOM	1758	CG	LYS	227	15.274	12.876	16.517	1.00	25.51
ATOM	1759	CD	LYS	227	15.905	13.931	15.600	1.00	27.52
ATOM	1760	CE	LYS	227	16.328	15.168	16.402	1.00	29.31
ATOM	1761	NZ	LYS	227	16.685	16.362	15.537	1.00	31.02
ATOM	1762	C	LYS	227	13.699	10.469	17.679	1.00	19.52
ATOM	1763	O	LYS	227	13.958	9.343	17.253	1.00	18.64
ATOM	1764	N	PHE	228	13.927	10.819	18.942	1.00	16.76
ATOM	1765	CA	PHE	228	14.549	9.850	19.842	1.00	15.71
ATOM	1766	CB	PHE	228	15.499	10.564	20.819	1.00	15.17
ATOM	1767	CG	PHE	228	16.624	11.311	20.129	1.00	16.25
ATOM	1768	CD1	PHE	228	16.691	12.697	20.190	1.00	15.63
ATOM	1769	CD2	PHE	228	17.572	10.626	19.369	1.00	16.44
ATOM	1770	CE1	PHE	228	17.683	13.407	19.501	1.00	16.18
ATOM	1771	CE2	PHE	228	18.575	11.325	18.668	1.00	17.04
ATOM	1772	CZ	PHE	228	18.626	12.716	18.737	1.00	16.02
ATOM	1773	C	PHE	228	13.607	8.907	20.596	1.00	14.94
ATOM	1774	O	PHE	228	14.061	8.082	21.392	1.00	13.74
ATOM	1775	N	ILE	229	12.308	9.008	20.332	1.00	15.12
ATOM	1776	CA	ILE	229	11.338	8.132	20.984	1.00	14.85
ATOM	1777	CB	ILE	229	9.895	8.654	20.757	1.00	16.56
ATOM	1778	CG2	ILE	229	8.932	7.488	20.503	1.00	18.80
ATOM	1779	CG1	ILE	229	9.456	9.485	21.962	1.00	18.56
ATOM	1780	CD1	ILE	229	10.394	10.579	22.311	1.00	19.84
ATOM	1781	C	ILE	229	11.487	6.718	20.427	1.00	14.53
ATOM	1782	O	ILE	229	11.577	6.532	19.213	1.00	14.38
ATOM	1783	N	LYS	230	11.520	5.729	21.321	1.00	13.12
ATOM	1784	CA	LYS	230	11.664	4.324	20.943	1.00	13.05
ATOM	1785	CB	LYS	230	12.185	3.523	22.149	1.00	15.51
ATOM	1786	CG	LYS	230	12.176	2.004	21.973	1.00	18.04
ATOM	1787	CD	LYS	230	12.239	1.286	23.330	1.00	19.77
ATOM	1788	CE	LYS	230	12.225	-.237	23.207	1.00	21.97
ATOM	1789	NZ	LYS	230	12.074	-.877	24.539	1.00	24.63
ATOM	1790	C	LYS	230	10.318	3.750	20.490	1.00	12.28
ATOM	1791	O	LYS	230	9.297	3.966	21.132	1.00	11.71
ATOM	1792	N	LEU	231	10.314	3.013	19.386	1.00	10.80
ATOM	1793	CA	LEU	231	9.082	2.410	18.904	1.00	9.97
ATOM	1794	CB	LEU	231	9.058	2.325	17.375	1.00	8.92
ATOM	1795	CG	LEU	231	7.756	1.784	16.750	1.00	8.48
ATOM	1796	CD1	LEU	231	6.597	2.693	17.143	1.00	8.56
ATOM	1797	CD2	LEU	231	7.871	1.718	15.216	1.00	9.36
ATOM	1798	C	LEU	231	9.041	1.009	19.487	1.00	10.07
ATOM	1799	O	LEU	231	10.021	.277	19.400	1.00	10.47
ATOM	1800	N	ASN	232	7.919	..654	20.104	1.00	8.98
ATOM	1801	CA	ASN	232	7.760	-.669	20.683	1.00	9.71
ATOM	1802	CB	ASN	232	6.415	-.764	21.415	1.00	10.54
ATOM	1803	CG	ASN	232	6.175	-2.135	22.003	1.00	10.95
ATOM	1804	OD1	ASN	232	6.889	-2.577	22.921	1.00	11.54
ATOM	1805	ND2	ASN	232	5.188	-2.831	21.466	1.00	10.91
ATOM	1806	C	ASN	232	7.812	-1.720	19.561	1.00	11.11
ATOM	1807	O	ASN	232	7.191	-1.549	18.504	1.00	11.77
ATOM	1808	N	GLN	233	8.566	-2.794	19.775	1.00	12.80
ATOM	1809	CA	GLN	233	8.649	-3.851	18.764	1.00	13.90
ATOM	1810	CB	GLN	233	10.082	-3.989	18.226	1.00	17.34
ATOM	1811	CG	GLN	233	10.453	-2.931	17.180	1.00	19.69
ATOM	1812	CD	GLN	233	9.365	-2.749	16.123	1.00	20.51

ATOM	1813	OE1	GLN	233	8.787	-3.723	15.635	1.00	22.00
ATOM	1814	NE2	GLN	233	9.086	-1.502	15.766	1.00	20.93
ATOM	1815	C	GLN	233	8.154	-5.201	19.269	1.00	13.98
ATOM	1816	O	GLN	233	8.048	-6.159	18.491	1.00	14.24
ATOM	1817	N	GLN	234	7.857	-5.286	20.564	1.00	12.74
ATOM	1818	CA	GLN	234	7.353	-6.529	21.148	1.00	12.31
ATOM	1819	CB	GLN	234	7.930	-6.755	22.549	1.00	15.33
ATOM	1820	CG	GLN	234	7.234	-7.864	23.306	1.00	18.33
ATOM	1821	CD	GLN	234	8.066	-8.407	24.459	1.00	19.33
ATOM	1822	OE1	GLN	234	8.728	-7.659	25.194	1.00	20.16
ATOM	1823	NE2	GLN	234	8.035	-9.716	24.624	1.00	21.28
ATOM	1824	C	GLN	234	5.833	-6.460	21.222	1.00	10.91
ATOM	1825	O	GLN	234	5.273	-5.652	21.964	1.00	10.50
ATOM	1826	N	PHE	235	5.168	-7.309	20.451	1.00	8.72
ATOM	1827	CA	PHE	235	3.708	-7.318	20.426	1.00	8.10
ATOM	1828	CB	PHE	235	3.189	-8.303	19.364	1.00	8.04
ATOM	1829	CG	PHE	235	1.684	-8.283	19.207	1.00	8.04
ATOM	1830	CD1	PHE	235	1.075	-7.438	18.275	1.00	7.52
ATOM	1831	CD2	PHE	235	.874	-9.047	20.047	1.00	7.89
ATOM	1832	CE1	PHE	235	-.320	-7.348	18.187	1.00	7.44
ATOM	1833	CE2	PHE	235	-.515	-8.966	19.972	1.00	7.63
ATOM	1834	CZ	PHE	235	-1.114	-8.110	19.038	1.00	7.53
ATOM	1835	C	PHE	235	3.093	-7.689	21.779	1.00	7.53
ATOM	1836	O	PHE	235	3.396	-8.747	22.329	1.00	8.01
ATOM	1837	N	VAL	236	2.224	-6.817	22.286	1.00	7.33
ATOM	1838	CA	VAL	236	1.502	-7.029	23.541	1.00	6.95
ATOM	1839	CB	VAL	236	1.596	-5.804	24.465	1.00	8.03
ATOM	1840	CG1	VAL	236	.687	-6.005	25.683	1.00	8.50
ATOM	1841	CG2	VAL	236	3.019	-5.609	24.920	1.00	7.89
ATOM	1842	C	VAL	236	.017	-7.278	23.241	1.00	7.38
ATOM	1843	O	VAL	236	-.624	-6.484	22.554	1.00	7.02
ATOM	1844	N	PRO	237	-.550	-8.390	23.745	1.00	7.48
ATOM	1845	CD	PRO	237	.076	-9.512	24.477	1.00	8.58
ATOM	1846	CA	PRO	237	-1.967	-8.666	23.478	1.00	7.09
ATOM	1847	CB	PRO	237	-2.051	-10.181	23.651	1.00	6.67
ATOM	1848	CG	PRO	237	-1.120	-10.418	24.798	1.00	7.16
ATOM	1849	C	PRO	237	-2.905	-7.913	24.426	1.00	7.37
ATOM	1850	O	PRO	237	-3.601	-8.510	25.248	1.00	6.71
ATOM	1851	N	PHE	238	-2.923	-6.591	24.303	1.00	6.84
ATOM	1852	CA	PHE	238	-3.757	-5.757	25.150	1.00	7.40
ATOM	1853	CB	PHE	238	-3.737	-4.302	24.669	1.00	7.33
ATOM	1854	CG	PHE	238	-2.427	-3.608	24.890	1.00	5.73
ATOM	1855	CD1	PHE	238	-1.540	-3.396	23.831	1.00	6.53
ATOM	1856	CD2	PHE	238	-2.088	-3.138	26.156	1.00	6.95
ATOM	1857	CE1	PHE	238	-.327	-2.715	24.038	1.00	5.83
ATOM	1858	CE2	PHE	238	-.882	-2.460	26.371	1.00	6.68
ATOM	1859	CZ	PHE	238	.000	-2.247	25.308	1.00	7.39
ATOM	1860	C	PHE	238	-5.207	-6.191	25.297	1.00	7.49
ATOM	1861	O	PHE	238	-5.779	-6.020	26.373	1.00	7.93
ATOM	1862	N	THR	239	-5.812	-6.745	24.243	1.00	7.66
ATOM	1863	CA	THR	239	-7.216	-7.150	24.350	1.00	8.17
ATOM	1864	CB	THR	239	-7.878	-7.480	22.974	1.00	7.45
ATOM	1865	OG1	THR	239	-7.189	-8.574	22.345	1.00	10.85
ATOM	1866	CG2	THR	239	-7.888	-6.240	22.056	1.00	8.40
ATOM	1867	C	THR	239	-7.412	-8.354	25.262	1.00	8.11
ATOM	1868	O	THR	239	-8.551	-8.725	25.573	1.00	8.54
ATOM	1869	N	GLN	240	-6.308	-8.959	25.689	1.00	8.14
ATOM	1870	CA	GLN	240	-6.373	-10.117	26.573	1.00	8.88
ATOM	1871	CB	GLN	240	-5.440	-11.226	26.075	1.00	9.09
ATOM	1872	CG	GLN	240	-5.704	-11.662	24.628	1.00	9.66

ATOM	1873	CD	GLN	240	-4.859	-12.855	24.217	1.00	10.41
ATOM	1874	OE1	GLN	240	-3.785	-13.100	24.784	1.00	12.02
ATOM	1875	NE2	GLN	240	-5.330	-13.600	23.211	1.00	11.48
ATOM	1876	C	GLN	240	-5.987	-9.739	27.996	1.00	9.93
ATOM	1877	O	GLN	240	-6.002	-10.579	28.899	1.00	10.08
ATOM	1878	N	LEU	241	-5.655	-8.470	28.195	1.00	8.44
ATOM	1879	CA	LEU	241	-5.240	-7.989	29.506	1.00	10.64
ATOM	1880	CB	LEU	241	-4.050	-7.036	29.346	1.00	9.65
ATOM	1881	CG	LEU	241	-2.908	-7.573	28.477	1.00	10.64
ATOM	1882	CD1	LEU	241	-1.764	-6.566	28.403	1.00	9.91
ATOM	1883	CD2	LEU	241	-2.419	-8.895	29.058	1.00	11.27
ATOM	1884	C	LEU	241	-6.360	-7.280	30.243	1.00	9.99
ATOM	1885	O	LEU	241	-7.315	-6.784	29.631	1.00	11.34
ATOM	1886	N	ASP	242	-6.234	-7.242	31.567	1.00	11.60
ATOM	1887	CA	ASP	242	-7.203	-6.569	32.418	1.00	11.57
ATOM	1888	CB	ASP	242	-7.255	-7.243	33.784	1.00	11.84
ATOM	1889	CG	ASP	242	-8.376	-6.713	34.641	1.00	14.30
ATOM	1890	OD1	ASP	242	-8.775	-5.539	34.436	1.00	14.28
ATOM	1891	OD2	ASP	242	-8.855	-7.464	35.522	1.00	15.01
ATOM	1892	C	ASP	242	-6.715	-5.132	32.593	1.00	11.02
ATOM	1893	O	ASP	242	-5.797	-4.882	33.371	1.00	11.18
ATOM	1894	N	LEU	243	-7.340	-4.197	31.884	1.00	10.51
ATOM	1895	CA	LEU	243	-6.945	-2.796	31.933	1.00	10.12
ATOM	1896	CB	LEU	243	-7.037	-2.179	30.532	1.00	11.64
ATOM	1897	CG	LEU	243	-6.287	-2.925	29.424	1.00	10.17
ATOM	1898	CD1	LEU	243	-6.420	-2.148	28.109	1.00	12.49
ATOM	1899	CD2	LEU	243	-4.822	-3.080	29.809	1.00	11.10
ATOM	1900	C	LEU	243	-7.794	-1.969	32.885	1.00	11.28
ATOM	1901	O	LEU	243	-7.782	-.744	32.800	1.00	11.62
ATOM	1902	N	SER	244	-8.512	-2.622	33.795	1.00	12.14
ATOM	1903	CA	SER	244	-9.370	-1.896	34.722	1.00	12.80
ATOM	1904	CB	SER	244	-10.173	-2.874	35.591	1.00	12.78
ATOM	1905	OG	SER	244	-9.326	-3.617	36.452	1.00	14.04
ATOM	1906	C	SER	244	-8.572	-.951	35.616	1.00	12.11
ATOM	1907	O	SER	244	-9.121	.033	36.130	1.00	12.65
ATOM	1908	N	TYR	245	-7.281	-1.239	35.798	1.00	10.44
ATOM	1909	CA	TYR	245	-6.438	-.399	36.637	1.00	9.18
ATOM	1910	CB	TYR	245	-5.037	-1.010	36.744	1.00	9.28
ATOM	1911	CG	TYR	245	-4.183	-.943	35.494	1.00	8.84
ATOM	1912	CD1	TYR	245	-3.291	.116	35.296	1.00	9.80
ATOM	1913	CE1	TYR	245	-2.442	.155	34.192	1.00	9.66
ATOM	1914	CD2	TYR	245	-4.212	-1.967	34.536	1.00	8.16
ATOM	1915	CE2	TYR	245	-3.363	-1.935	33.416	1.00	7.89
ATOM	1916	CZ	TYR	245	-2.479	-.870	33.257	1.00	8.95
ATOM	1917	OH	TYR	245	-1.620	-.830	32.179	1.00	7.59
ATOM	1918	C	TYR	245	-6.372	1.045	36.108	1.00	9.25
ATOM	1919	O	TYR	245	-5.989	1.965	36.834	1.00	7.87
ATOM	1920	N	LEU	246	-6.752	1.239	34.844	1.00	8.87
ATOM	1921	CA	LEU	246	-6.747	2.569	34.257	1.00	9.77
ATOM	1922	CB	LEU	246	-6.529	2.477	32.735	1.00	9.71
ATOM	1923	CG	LEU	246	-5.128	2.015	32.300	1.00	10.16
ATOM	1924	CD1	LEU	246	-5.121	1.763	30.806	1.00	9.59
ATOM	1925	CD2	LEU	246	-4.084	3.060	32.667	1.00	10.13
ATOM	1926	C	LEU	246	-8.002	3.405	34.575	1.00	10.93
ATOM	1927	O	LEU	246	-8.008	4.618	34.341	1.00	10.86
ATOM	1928	N	GLN	247	-9.059	2.793	35.116	1.00	12.45
ATOM	1929	CA	GLN	247	-10.237	3.608	35.446	1.00	13.63
ATOM	1930	CB	GLN	247	-11.391	2.748	35.958	1.00	18.20
ATOM	1931	CG	GLN	247	-12.372	2.324	34.850	1.00	22.31
ATOM	1932	CD	GLN	247	-13.285	3.474	34.370	1.00	24.50

ATOM	1933	OE1	GLN	247	-13.247	4.592	34.912	1.00	24.67
ATOM	1934	NE2	GLN	247	-14.119	3.193	33.365	1.00	25.70
ATOM	1935	C	GLN	247	-9.836	4.646	36.484	1.00	12.81
ATOM	1936	O	GLN	247	-9.048	4.366	37.380	1.00	10.85
ATOM	1937	N	GLN	248	-10.373	5.854	36.360	1.00	13.19
ATOM	1938	CA	GLN	248	-10.012	6.937	37.268	1.00	14.45
ATOM	1939	CB	GLN	248	-10.878	8.173	36.993	1.00	16.12
ATOM	1940	CG	GLN	248	-10.318	9.449	37.634	1.00	17.45
ATOM	1941	CD	GLN	248	-11.248	10.661	37.527	1.00	17.90
ATOM	1942	OE1	GLN	248	-12.400	10.621	37.967	1.00	19.24
ATOM	1943	NE2	GLN	248	-10.739	11.749	36.964	1.00	17.81
ATOM	1944	C	GLN	248	-10.020	6.629	38.766	1.00	14.49
ATOM	1945	O	GLN	248	-9.058	6.957	39.469	1.00	13.95
ATOM	1946	N	GLU	249	-11.089	6.000	39.262	1.00	15.61
ATOM	1947	CA	GLU	249	-11.171	5.700	40.686	1.00	17.13
ATOM	1948	CB	GLU	249	-12.562	5.120	41.056	1.00	20.18
ATOM	1949	CG	GLU	249	-13.058	3.855	40.325	1.00	23.71
ATOM	1950	CD	GLU	249	-13.718	4.136	38.977	1.00	26.08
ATOM	1951	OE1	GLU	249	-14.319	3.194	38.396	1.00	26.94
ATOM	1952	OE2	GLU	249	-13.650	5.295	38.493	1.00	27.25
ATOM	1953	C	GLU	249	-10.027	4.794	41.177	1.00	16.89
ATOM	1954	O	GLU	249	-9.414	5.072	42.224	1.00	17.95
ATOM	1955	N	ALA	250	-9.706	3.740	40.424	1.00	14.79
ATOM	1956	CA	ALA	250	-8.619	2.841	40.824	1.00	13.69
ATOM	1957	CB	ALA	250	-8.711	1.528	40.039	1.00	12.34
ATOM	1958	C	ALA	250	-7.225	3.467	40.645	1.00	12.45
ATOM	1959	O	ALA	250	-6.370	3.380	41.528	1.00	11.64
ATOM	1960	N	TYR	251	-7.014	4.129	39.516	1.00	11.68
ATOM	1961	CA	TYR	251	-5.726	4.738	39.222	1.00	10.57
ATOM	1962	CB	TYR	251	-5.756	5.367	37.827	1.00	8.98
ATOM	1963	CG	TYR	251	-4.392	5.612	37.228	1.00	7.93
ATOM	1964	CD1	TYR	251	-3.723	4.594	36.545	1.00	7.65
ATOM	1965	CE1	TYR	251	-2.463	4.806	35.987	1.00	7.45
ATOM	1966	CD2	TYR	251	-3.766	6.853	37.346	1.00	7.80
ATOM	1967	CE2	TYR	251	-2.505	7.081	36.795	1.00	7.13
ATOM	1968	CZ	TYR	251	-1.858	6.056	36.115	1.00	6.53
ATOM	1969	OH	TYR	251	-.608	6.277	35.568	1.00	6.58
ATOM	1970	C	TYR	251	-5.356	5.807	40.237	1.00	10.74
ATOM	1971	O	TYR	251	-4.257	5.812	40.806	1.00	10.67
ATOM	1972	N	ASP	252	-6.292	6.721	40.453	1.00	11.98
ATOM	1973	CA	ASP	252	-6.077	7.832	41.369	1.00	13.40
ATOM	1974	CB	ASP	252	-7.234	8.820	41.254	1.00	13.73
ATOM	1975	CG	ASP	252	-7.117	9.682	40.024	1.00	14.25
ATOM	1976	OD1	ASP	252	-6.184	9.414	39.242	1.00	12.81
ATOM	1977	OD2	ASP	252	-7.933	10.618	39.831	1.00	15.62
ATOM	1978	C	ASP	252	-5.859	7.446	42.809	1.00	14.64
ATOM	1979	O	ASP	252	-5.435	8.271	43.622	1.00	16.34
ATOM	1980	N	ARG	253	-6.163	6.200	43.127	1.00	14.66
ATOM	1981	CA	ARG	253	-5.961	5.692	44.470	1.00	15.70
ATOM	1982	CB	ARG	253	-7.124	4.795	44.878	1.00	17.79
ATOM	1983	CG	ARG	253	-6.914	4.135	46.219	1.00	21.56
ATOM	1984	CD	ARG	253	-8.096	3.253	46.592	1.00	24.09
ATOM	1985	NE	ARG	253	-7.693	1.860	46.703	1.00	28.71
ATOM	1986	CZ	ARG	253	-7.344	1.094	45.675	1.00	30.19
ATOM	1987	NH1	ARG	253	-7.361	1.596	44.448	1.00	31.14
ATOM	1988	NH2	ARG	253	-6.953	-.167	45.887	1.00	31.53
ATOM	1989	C	ARG	253	-4.663	4.890	44.478	1.00	14.76
ATOM	1990	O	ARG	253	-3.750	5.174	45.253	1.00	13.88
ATOM	1991	N	ASP	254	-4.568	3.901	43.590	1.00	14.63
ATOM	1992	CA	ASP	254	-3.378	3.058	43.548	1.00	14.64

ATOM	1993	CB	ASP	254	-3.670	1.772	42.759	1.00	16.43
ATOM	1994	CG	ASP	254	-4.677	.864	43.467	1.00	18.49
ATOM	1995	OD1	ASP	254	-4.863	1.020	44.695	1.00	19.22
ATOM	1996	OD2	ASP	254	-5.271	-.024	42.812	1.00	18.69
ATOM	1997	C	ASP	254	-2.097	3.719	43.021	1.00	13.66
ATOM	1998	O	ASP	254	-1.040	3.615	43.636	1.00	13.68
ATOM	1999	N	PHE	255	-2.171	4.405	41.887	1.00	13.59
ATOM	2000	CA	PHE	255	-.966	5.035	41.370	1.00	13.77
ATOM	2001	CB	PHE	255	-1.209	5.613	39.970	1.00	13.03
ATOM	2002	CG	PHE	255	.057	5.995	39.263	1.00	12.97
ATOM	2003	CD1	PHE	255	.944	5.011	38.834	1.00	12.71
ATOM	2004	CD2	PHE	255	.403	7.330	39.097	1.00	11.88
ATOM	2005	CE1	PHE	255	2.170	5.361	38.246	1.00	12.10
ATOM	2006	CE2	PHE	255	1.630	7.694	38.510	1.00	11.62
ATOM	2007	CZ	PHE	255	2.510	6.709	38.086	1.00	10.32
ATOM	2008	C	PHE	255	-.449	6.130	42.309	1.00	14.17
ATOM	2009	O	PHE	255	.757	6.234	42.560	1.00	13.00
ATOM	2010	N	LEU	256	-1.355	6.939	42.850	1.00	14.47
ATOM	2011	CA	LEU	256	-.964	8.009	43.761	1.00	15.21
ATOM	2012	CB	LEU	256	-2.168	8.896	44.089	1.00	16.52
ATOM	2013	CG	LEU	256	-2.535	9.999	43.087	1.00	17.89
ATOM	2014	CD1	LEU	256	-1.496	11.115	43.163	1.00	18.37
ATOM	2015	CD2	LEU	256	-2.618	9.439	41.679	1.00	19.32
ATOM	2016	C	LEU	256	-.348	7.488	45.055	1.00	15.25
ATOM	2017	O	LEU	256	.645	8.034	45.551	1.00	14.40
ATOM	2018	N	ALA	257	-.953	6.446	45.613	1.00	14.11
ATOM	2019	CA	ALA	257	-.430	5.851	46.835	1.00	14.22
ATOM	2020	CB	ALA	257	-1.375	4.761	47.351	1.00	15.00
ATOM	2021	C	ALA	257	.947	5.263	46.526	1.00	14.36
ATOM	2022	O	ALA	257	1.834	5.251	47.383	1.00	12.87
ATOM	2023	N	ARG	258	1.128	4.774	45.300	1.00	14.11
ATOM	2024	CA	ARG	258	2.419	4.226	44.908	1.00	13.47
ATOM	2025	CB	ARG	258	2.344	3.564	43.541	1.00	16.19
ATOM	2026	CG	ARG	258	3.715	3.192	43.038	1.00	19.25
ATOM	2027	CD	ARG	258	4.278	2.007	43.793	1.00	22.51
ATOM	2028	NE	ARG	258	3.652	.747	43.389	1.00	24.68
ATOM	2029	CZ	ARG	258	3.568	.339	42.125	1.00	25.98
ATOM	2030	NH1	ARG	258	4.070	1.097	41.163	1.00	27.05
ATOM	2031	NH2	ARG	258	2.972	-.803	41.825	1.00	25.34
ATOM	2032	C	ARG	258	3.476	5.322	44.831	1.00	12.98
ATOM	2033	O	ARG	258	4.588	5.177	45.342	1.00	12.00
ATOM	2034	N	VAL	259	3.126	6.417	44.164	1.00	12.20
ATOM	2035	CA	VAL	259	4.051	7.535	44.007	1.00	12.73
ATOM	2036	CB	VAL	259	3.418	8.632	43.108	1.00	11.07
ATOM	2037	CG1	VAL	259	4.256	9.940	43.141	1.00	12.10
ATOM	2038	CG2	VAL	259	3.279	8.093	41.696	1.00	11.85
ATOM	2039	C	VAL	259	4.455	8.143	45.345	1.00	11.73
ATOM	2040	O	VAL	259	5.641	8.315	45.629	1.00	11.99
ATOM	2041	N	TYR	260	3.481	8.464	46.182	1.00	12.62
ATOM	2042	CA	TYR	260	3.831	9.077	47.451	1.00	12.68
ATOM	2043	CB	TYR	260	2.680	9.966	47.945	1.00	13.38
ATOM	2044	CG	TYR	260	2.524	11.197	47.056	1.00	11.91
ATOM	2045	CD1	TYR	260	1.598	11.220	46.007	1.00	11.34
ATOM	2046	CE1	TYR	260	1.556	12.288	45.098	1.00	11.06
ATOM	2047	CD2	TYR	260	3.400	12.281	47.182	1.00	12.97
ATOM	2048	CE2	TYR	260	3.368	13.349	46.281	1.00	12.11
ATOM	2049	CZ	TYR	260	2.450	13.348	45.241	1.00	11.20
ATOM	2050	OH	TYR	260	2.471	14.396	44.341	1.00	10.67
ATOM	2051	C	TYR	260	4.310	8.078	48.506	1.00	13.85
ATOM	2052	O	TYR	260	4.895	8.469	49.516	1.00	14.94

ATOM	2053	N	GLY	261	4.102	6.792	48.240	1.00	14.25
ATOM	2054	CA	GLY	261	4.548	5.758	49.156	1.00	15.09
ATOM	2055	C	GLY	261	6.019	5.444	48.918	1.00	15.37
ATOM	2056	O	GLY	261	6.694	4.839	49.762	1.00	15.58
ATOM	2057	N	ALA	262	6.524	5.834	47.749	1.00	15.87
ATOM	2058	CA	ALA	262	7.922	5.596	47.418	1.00	16.56
ATOM	2059	CB	ALA	262	8.136	5.769	45.937	1.00	16.86
ATOM	2060	C	ALA	262	8.848	6.540	48.187	1.00	17.88
ATOM	2061	O	ALA	262	8.500	7.697	48.463	1.00	19.24
ATOM	2062	N	PRO	263	10.045	6.058	48.546	1.00	17.58
ATOM	2063	CD	PRO	263	10.657	4.758	48.228	1.00	18.05
ATOM	2064	CA	PRO	263	10.982	6.907	49.280	1.00	18.21
ATOM	2065	CB	PRO	263	12.149	5.955	49.561	1.00	17.95
ATOM	2066	CG	PRO	263	12.134	5.051	48.367	1.00	18.74
ATOM	2067	C	PRO	263	11.388	8.138	48.465	1.00	18.31
ATOM	2068	O	PRO	263	11.477	8.084	47.233	1.00	17.32
ATOM	2069	N	GLN	264	11.605	9.250	49.164	1.00	18.19
ATOM	2070	CA	GLN	264	12.017	10.509	48.557	1.00	18.34
ATOM	2071	CB	GLN	264	11.461	11.684	49.372	1.00	19.05
ATOM	2072	CG	GLN	264	11.483	13.019	48.650	1.00	20.04
ATOM	2073	CD	GLN	264	10.702	14.124	49.371	1.00	20.34
ATOM	2074	OE1	GLN	264	9.536	13.942	49.757	1.00	21.60
ATOM	2075	NE2	GLN	264	11.334	15.281	49.529	1.00	19.44
ATOM	2076	C	GLN	264	13.548	10.587	48.510	1.00	18.12
ATOM	2077	O	GLN	264	14.232	10.232	49.478	1.00	18.53
ATOM	2078	N	LEU	265	14.088	11.021	47.376	1.00	16.76
ATOM	2079	CA	LEU	265	15.536	11.170	47.216	1.00	17.44
ATOM	2080	CB	LEU	265	16.106	10.090	46.292	1.00	17.05
ATOM	2081	CG	LEU	265	16.567	8.758	46.898	1.00	17.70
ATOM	2082	CD1	LEU	265	15.392	8.066	47.586	1.00	18.87
ATOM	2083	CD2	LEU	265	17.160	7.873	45.783	1.00	15.97
ATOM	2084	C	LEU	265	15.810	12.538	46.599	1.00	18.35
ATOM	2085	O	LEU	265	14.979	13.049	45.829	1.00	17.65
ATOM	2086	N	GLN	266	16.958	13.125	46.942	1.00	18.61
ATOM	2087	CA	GLN	266	17.383	14.425	46.413	1.00	19.40
ATOM	2088	CB	GLN	266	18.689	14.897	47.089	1.00	23.72
ATOM	2089	CG	GLN	266	18.665	14.994	48.621	1.00	28.87
ATOM	2090	CD	GLN	266	20.068	14.941	49.246	1.00	31.36
ATOM	2091	OE1	GLN	266	20.917	15.838	49.041	1.00	33.08
ATOM	2092	NE2	GLN	266	20.322	13.880	50.009	1.00	32.71
ATOM	2093	C	GLN	266	17.682	14.174	44.939	1.00	19.22
ATOM	2094	O	GLN	266	18.243	13.125	44.592	1.00	17.61
ATOM	2095	N	VAL	267	17.347	15.129	44.076	1.00	17.99
ATOM	2096	CA	VAL	267	17.599	14.949	42.644	1.00	18.22
ATOM	2097	CB	VAL	267	17.174	16.216	41.833	1.00	18.19
ATOM	2098	CG1	VAL	267	18.047	17.417	42.205	1.00	17.79
ATOM	2099	CG2	VAL	267	17.259	15.923	40.332	1.00	18.95
ATOM	2100	C	VAL	267	19.063	14.586	42.333	1.00	19.35
ATOM	2101	O	VAL	267	19.338	13.777	41.433	1.00	18.55
ATOM	2102	N	GLU	268	20.008	15.145	43.085	1.00	21.63
ATOM	2103	CA	GLU	268	21.422	14.843	42.828	1.00	22.92
ATOM	2104	CB	GLU	268	22.321	15.841	43.577	1.00	28.85
ATOM	2105	CG	GLU	268	22.409	17.218	42.886	1.00	34.76
ATOM	2106	CD	GLU	268	22.259	18.393	43.842	1.00	38.05
ATOM	2107	OE1	GLU	268	22.933	18.396	44.902	1.00	40.90
ATOM	2108	OE2	GLU	268	21.466	19.330	43.534	1.00	40.14
ATOM	2109	C	GLU	268	21.821	13.401	43.147	1.00	22.41
ATOM	2110	O	GLU	268	22.775	12.880	42.560	1.00	21.23
ATOM	2111	N	LYS	269	21.097	12.743	44.053	1.00	21.49
ATOM	2112	CA	LYS	269	21.394	11.348	44.382	1.00	20.55

ATOM	2113	CB	LYS	269	20.846	10.972	45.759	1.00	22.53
ATOM	2114	CG	LYS	269	21.527	11.731	46.872	1.00	23.87
ATOM	2115	CD	LYS	269	21.499	10.973	48.170	1.00	26.41
ATOM	2116	CE	LYS	269	22.330	11.732	49.200	1.00	27.52
ATOM	2117	NZ	LYS	269	22.207	11.146	50.566	1.00	30.38
ATOM	2118	C	LYS	269	20.837	10.416	43.315	1.00	19.98
ATOM	2119	O	LYS	269	21.381	9.332	43.064	1.00	19.43
ATOM	2120	N	VAL	270	19.742	10.831	42.679	1.00	18.28
ATOM	2121	CA	VAL	270	19.189	10.034	41.603	1.00	17.73
ATOM	2122	CB	VAL	270	17.787	10.517	41.221	1.00	16.04
ATOM	2123	CG1	VAL	270	17.338	9.825	39.956	1.00	15.32
ATOM	2124	CG2	VAL	270	16.820	10.227	42.356	1.00	14.25
ATOM	2125	C	VAL	270	20.128	10.199	40.404	1.00	18.75
ATOM	2126	O	VAL	270	20.531	9.218	39.782	1.00	17.62
ATOM	2127	N	ARG	271	20.482	11.444	40.103	1.00	20.39
ATOM	2128	CA	ARG	271	21.360	11.736	38.976	1.00	22.65
ATOM	2129	CB	ARG	271	21.674	13.242	38.936	1.00	25.53
ATOM	2130	CG	ARG	271	22.102	13.733	37.567	1.00	28.90
ATOM	2131	CD	ARG	271	23.111	14.902	37.597	1.00	31.40
ATOM	2132	NE	ARG	271	22.612	16.107	38.261	1.00	35.06
ATOM	2133	CZ	ARG	271	23.280	17.261	38.352	1.00	37.24
ATOM	2134	NH1	ARG	271	24.496	17.398	37.817	1.00	38.39
ATOM	2135	NH2	ARG	271	22.729	18.291	38.989	1.00	37.97
ATOM	2136	C	ARG	271	22.665	10.925	39.086	1.00	23.29
ATOM	2137	O	ARG	271	23.149	10.357	38.094	1.00	22.94
ATOM	2138	N	THR	272	23.214	10.843	40.296	1.00	24.37
ATOM	2139	CA	THR	272	24.480	10.135	40.514	1.00	24.57
ATOM	2140	CB	THR	272	25.270	10.810	41.662	1.00	26.25
ATOM	2141	OG1	THR	272	25.706	12.121	41.236	1.00	27.68
ATOM	2142	CG2	THR	272	26.493	9.969	42.048	1.00	26.59
ATOM	2143	C	THR	272	24.345	8.625	40.764	1.00	24.47
ATOM	2144	O	THR	272	25.337	7.896	40.903	1.00	24.47
ATOM	2145	N	ASN	273	23.110	8.155	40.798	1.00	24.12
ATOM	2146	CA	ASN	273	22.807	6.739	40.997	1.00	23.87
ATOM	2147	CB	ASN	273	23.486	5.900	39.907	1.00	23.17
ATOM	2148	CG	ASN	273	22.580	4.802	39.386	1.00	22.43
ATOM	2149	OD1	ASN	273	21.357	4.923	39.467	1.00	22.11
ATOM	2150	ND2	ASN	273	23.161	3.732	38.843	1.00	21.43
ATOM	2151	C	ASN	273	23.170	6.232	42.392	1.00	24.72
ATOM	2152	O	ASN	273	23.836	5.196	42.565	1.00	24.24
ATOM	2153	N	ASP	274	22.705	6.984	43.387	1.00	24.55
ATOM	2154	CA	ASP	274	22.899	6.678	44.799	1.00	24.36
ATOM	2155	CB	ASP	274	22.869	7.964	45.616	1.00	27.85
ATOM	2156	CG	ASP	274	24.086	8.124	46.479	1.00	29.93
ATOM	2157	OD1	ASP	274	24.351	7.238	47.333	1.00	30.74
ATOM	2158	OD2	ASP	274	24.801	9.138	46.290	1.00	32.19
ATOM	2159	C	ASP	274	21.769	5.787	45.282	1.00	23.44
ATOM	2160	O	ASP	274	20.681	5.782	44.698	1.00	22.19
ATOM	2161	N	ARG	275	22.027	5.029	46.348	1.00	21.69
ATOM	2162	CA	ARG	275	21.000	4.175	46.919	1.00	20.61
ATOM	2163	CB	ARG	275	19.956	5.056	47.608	1.00	20.79
ATOM	2164	CG	ARG	275	20.557	6.114	48.530	1.00	21.46
ATOM	2165	CD	ARG	275	21.016	5.432	49.785	1.00	21.63
ATOM	2166	NE	ARG	275	19.914	4.688	50.396	1.00	21.94
ATOM	2167	CZ	ARG	275	18.974	5.232	51.164	1.00	22.83
ATOM	2168	NH1	ARG	275	19.011	6.534	51.427	1.00	23.76
ATOM	2169	NH2	ARG	275	17.982	4.483	51.638	1.00	22.90
ATOM	2170	C	ARG	275	20.321	3.336	45.845	1.00	19.82
ATOM	2171	O	ARG	275	19.090	3.402	45.690	1.00	20.00
ATOM	2172	N	LYS	276	21.101	2.536	45.127	1.00	19.25

ATOM	2173	CA	LYS	276	20.551	1.704	44.059	1.00	18.65
ATOM	2174	CB	LYS	276	21.674	1.064	43.231	1.00	20.17
ATOM	2175	CG	LYS	276	22.391	2.036	42.287	1.00	21.99
ATOM	2176	CD	LYS	276	23.685	1.444	41.713	1.00	23.67
ATOM	2177	CE	LYS	276	23.517	-.013	41.236	1.00	25.59
ATOM	2178	NZ	LYS	276	22.795	-.126	39.929	1.00	27.35
ATOM	2179	C	LYS	276	19.591	.620	44.521	1.00	17.84
ATOM	2180	O	LYS	276	18.912	.010	43.700	1.00	17.03
ATOM	2181	N	GLU	277	19.541	.354	45.822	1.00	15.97
ATOM	2182	CA	GLU	277	18.629	-.659	46.337	1.00	15.31
ATOM	2183	CB	GLU	277	18.953	-.987	47.802	1.00	14.14
ATOM	2184	CG	GLU	277	18.649	.135	48.784	1.00	15.21
ATOM	2185	CD	GLU	277	19.821	1.068	49.032	1.00	15.40
ATOM	2186	OE1	GLU	277	20.744	1.164	48.189	1.00	15.55
ATOM	2187	OE2	GLU	277	19.817	1.726	50.097	1.00	16.99
ATOM	2188	C	GLU	277	17.187	-.166	46.222	1.00	15.45
ATOM	2189	O	GLU	277	16.240	-.958	46.276	1.00	15.78
ATOM	2190	N	LEU	278	17.012	1.145	46.062	1.00	15.24
ATOM	2191	CA	LEU	278	15.674	1.712	45.931	1.00	15.47
ATOM	2192	CB	LEU	278	15.644	3.144	46.487	1.00	15.54
ATOM	2193	CG	LEU	278	16.187	3.346	47.907	1.00	15.99
ATOM	2194	CD1	LEU	278	16.125	4.830	48.242	1.00	15.73
ATOM	2195	CD2	LEU	278	15.393	2.539	48.911	1.00	16.98
ATOM	2196	C	LEU	278	15.326	1.717	44.448	1.00	14.95
ATOM	2197	O	LEU	278	15.736	2.610	43.723	1.00	16.11
ATOM	2198	N	GLY	279	14.574	.715	44.004	1.00	15.41
ATOM	2199	CA	GLY	279	14.214	.620	42.597	1.00	14.73
ATOM	2200	C	GLY	279	13.120	1.571	42.123	1.00	13.97
ATOM	2201	O	GLY	279	12.839	1.647	40.935	1.00	14.12
ATOM	2202	N	GLU	280	12.481	2.277	43.041	1.00	13.50
ATOM	2203	CA	GLU	280	11.432	3.216	42.674	1.00	13.24
ATOM	2204	CB	GLU	280	10.062	2.524	42.692	1.00	14.95
ATOM	2205	CG	GLU	280	8.870	3.432	42.358	1.00	16.42
ATOM	2206	CD	GLU	280	7.595	2.649	42.061	1.00	17.87
ATOM	2207	OE1	GLU	280	7.483	1.483	42.492	1.00	19.78
ATOM	2208	OE2	GLU	280	6.691	3.199	41.400	1.00	16.28
ATOM	2209	C	GLU	280	11.503	4.302	43.714	1.00	12.86
ATOM	2210	O	GLU	280	11.377	4.039	44.909	1.00	13.56
ATOM	2211	N	VAL	281	11.710	5.527	43.254	1.00	12.54
ATOM	2212	CA	VAL	281	11.825	6.659	44.147	1.00	12.49
ATOM	2213	CB	VAL	281	13.281	7.088	44.283	1.00	12.53
ATOM	2214	CG1	VAL	281	14.142	5.886	44.695	1.00	13.91
ATOM	2215	CG2	VAL	281	13.765	7.669	42.941	1.00	13.87
ATOM	2216	C	VAL	281	11.062	7.873	43.663	1.00	12.53
ATOM	2217	O	VAL	281	10.603	7.943	42.524	1.00	12.06
ATOM	2218	N	ARG	282	10.986	8.858	44.540	1.00	12.80
ATOM	2219	CA	ARG	282	10.309	10.096	44.232	1.00	12.90
ATOM	2220	CB	ARG	282	9.106	10.236	45.150	1.00	14.21
ATOM	2221	CG	ARG	282	8.184	11.384	44.867	1.00	16.39
ATOM	2222	CD	ARG	282	6.874	11.110	45.572	1.00	17.31
ATOM	2223	NE	ARG	282	7.096	10.551	46.904	1.00	20.90
ATOM	2224	CZ	ARG	282	7.368	11.281	47.977	1.00	20.88
ATOM	2225	NH1	ARG	282	7.450	12.595	47.870	1.00	22.75
ATOM	2226	NH2	ARG	282	7.555	10.702	49.155	1.00	21.56
ATOM	2227	C	ARG	282	11.231	11.292	44.388	1.00	13.70
ATOM	2228	O	ARG	282	11.935	11.420	45.379	1.00	13.26
ATOM	2229	N	VAL	283	11.247	12.165	43.387	1.00	12.21
ATOM	2230	CA	VAL	283	12.047	13.381	43.467	1.00	11.81
ATOM	2231	CB	VAL	283	12.935	13.582	42.220	1.00	12.08
ATOM	2232	CG1	VAL	283	13.686	14.884	42.331	1.00	12.65

ATOM	2233	CG2	VAL	283	13.926	12.427	42.090	1.00	12.60
ATOM	2234	C	VAL	283	10.973	14.461	43.544	1.00	12.08
ATOM	2235	O	VAL	283	10.205	14.640	42.617	1.00	10.30
ATOM	2236	N	GLN	284	10.910	15.150	44.670	1.00	12.81
ATOM	2237	CA	GLN	284	9.900	16.170	44.883	1.00	14.43
ATOM	2238	CB	GLN	284	9.567	16.222	46.381	1.00	18.36
ATOM	2239	CG	GLN	284	8.147	16.669	46.728	1.00	22.58
ATOM	2240	CD	GLN	284	7.227	15.485	47.020	1.00	24.25
ATOM	2241	OE1	GLN	284	6.962	14.652	46.146	1.00	24.53
ATOM	2242	NE2	GLN	284	6.731	15.405	48.255	1.00	25.09
ATOM	2243	C	GLN	284	10.329	17.556	44.391	1.00	13.90
ATOM	2244	O	GLN	284	11.479	17.967	44.572	1.00	15.31
ATOM	2245	N	TYR	285	9.426	18.256	43.714	1.00	12.35
ATOM	2246	CA	TYR	285	9.713	19.613	43.272	1.00	12.75
ATOM	2247	CB	TYR	285	9.634	19.752	41.740	1.00	11.75
ATOM	2248	CG	TYR	285	8.270	19.519	41.121	1.00	10.30
ATOM	2249	CD1	TYR	285	7.294	20.514	41.138	1.00	9.91
ATOM	2250	CE1	TYR	285	6.055	20.319	40.530	1.00	9.63
ATOM	2251	CD2	TYR	285	7.970	18.313	40.484	1.00	8.51
ATOM	2252	CE2	TYR	285	6.731	18.102	39.878	1.00	9.24
ATOM	2253	CZ	TYR	285	5.780	19.114	39.906	1.00	9.82
ATOM	2254	OH	TYR	285	4.552	18.917	39.324	1.00	8.98
ATOM	2255	C	TYR	285	8.689	20.506	43.955	1.00	13.68
ATOM	2256	O	TYR	285	7.611	20.048	44.333	1.00	14.60
ATOM	2257	N	THR	286	9.026	21.773	44.143	1.00	14.62
ATOM	2258	CA	THR	286	8.099	22.674	44.791	1.00	16.92
ATOM	2259	CB	THR	286	8.780	23.397	45.991	1.00	17.92
ATOM	2260	OG1	THR	286	9.983	24.055	45.572	1.00	19.07
ATOM	2261	CG2	THR	286	9.138	22.378	47.071	1.00	17.79
ATOM	2262	C	THR	286	7.535	23.660	43.771	1.00	17.73
ATOM	2263	O	THR	286	6.394	23.517	43.328	1.00	20.09
ATOM	2264	N	GLY	287	8.336	24.627	43.363	1.00	18.37
ATOM	2265	CA	GLY	287	7.863	25.603	42.393	1.00	16.80
ATOM	2266	C	GLY	287	8.293	25.343	40.957	1.00	17.08
ATOM	2267	O	GLY	287	9.017	24.395	40.660	1.00	16.51
ATOM	2268	N	ARG	288	7.836	26.205	40.056	1.00	15.12
ATOM	2269	CA	ARG	288	8.156	26.111	38.643	1.00	15.02
ATOM	2270	CB	ARG	288	7.580	27.336	37.919	1.00	15.97
ATOM	2271	CG	ARG	288	8.147	28.676	38.412	1.00	18.54
ATOM	2272	CD	ARG	288	7.237	29.843	38.003	1.00	19.07
ATOM	2273	NE	ARG	288	6.020	29.938	38.818	1.00	20.83
ATOM	2274	CZ	ARG	288	4.918	30.571	38.427	1.00	21.71
ATOM	2275	NH1	ARG	288	4.896	31.154	37.237	1.00	22.64
ATOM	2276	NH2	ARG	288	3.836	30.618	39.207	1.00	22.44
ATOM	2277	C	ARG	288	9.671	26.022	38.415	1.00	14.57
ATOM	2278	O	ARG	288	10.134	25.257	37.577	1.00	12.10
ATOM	2279	N	ASP	289	10.442	26.805	39.165	1.00	14.61
ATOM	2280	CA	ASP	289	11.900	26.801	39.029	1.00	15.43
ATOM	2281	CB	ASP	289	12.515	27.883	39.909	1.00	19.34
ATOM	2282	CG	ASP	289	12.240	29.281	39.383	1.00	22.34
ATOM	2283	OD1	ASP	289	11.244	29.478	38.642	1.00	24.46
ATOM	2284	OD2	ASP	289	13.019	30.201	39.719	1.00	24.63
ATOM	2285	C	ASP	289	12.532	25.456	39.360	1.00	15.06
ATOM	2286	O	ASP	289	13.419	24.985	38.629	1.00	15.15
ATOM	2287	N	SER	290	12.078	24.836	40.451	1.00	13.91
ATOM	2288	CA	SER	290	12.606	23.537	40.836	1.00	13.23
ATOM	2289	CB	SER	290	12.242	23.193	42.293	1.00	11.59
ATOM	2290	OG	SER	290	10.844	23.106	42.483	1.00	13.58
ATOM	2291	C	SER	290	12.126	22.442	39.877	1.00	12.76
ATOM	2292	O	SER	290	12.821	21.451	39.658	1.00	13.20

ATOM	2293	N	PHE	291	10.952	22.614	39.277	1.00	12.92
ATOM	2294	CA	PHE	291	10.503	21.596	38.340	1.00	12.36
ATOM	2295	CB	PHE	291	9.066	21.844	37.897	1.00	11.24
ATOM	2296	CG	PHE	291	8.676	21.026	36.712	1.00	11.56
ATOM	2297	CD1	PHE	291	8.401	19.674	36.853	1.00	11.79
ATOM	2298	CD2	PHE	291	8.696	21.575	35.433	1.00	11.61
ATOM	2299	CE1	PHE	291	8.157	18.865	35.736	1.00	11.61
ATOM	2300	CE2	PHE	291	8.455	20.778	34.308	1.00	12.86
ATOM	2301	CZ	PHE	291	8.187	19.423	34.461	1.00	11.50
ATOM	2302	C	PHE	291	11.406	21.602	37.106	1.00	13.06
ATOM	2303	O	PHE	291	11.842	20.555	36.634	1.00	12.14
ATOM	2304	N	LYS	292	11.664	22.788	36.565	1.00	14.62
ATOM	2305	CA	LYS	292	12.511	22.893	35.384	1.00	14.66
ATOM	2306	CB	LYS	292	12.560	24.331	34.895	1.00	17.77
ATOM	2307	CG	LYS	292	11.218	24.889	34.566	1.00	21.15
ATOM	2308	CD	LYS	292	11.343	26.074	33.629	1.00	24.11
ATOM	2309	CE	LYS	292	10.033	26.290	32.888	1.00	25.78
ATOM	2310	NZ	LYS	292	10.161	27.302	31.807	1.00	27.65
ATOM	2311	C	LYS	292	13.923	22.435	35.682	1.00	14.83
ATOM	2312	O	LYS	292	14.553	21.746	34.884	1.00	14.54
ATOM	2313	N	ALA	293	14.422	22.827	36.843	1.00	13.35
ATOM	2314	CA	ALA	293	15.772	22.465	37.230	1.00	13.59
ATOM	2315	CB	ALA	293	16.104	23.110	38.569	1.00	13.94
ATOM	2316	C	ALA	293	15.936	20.948	37.328	1.00	13.03
ATOM	2317	O	ALA	293	16.868	20.365	36.755	1.00	13.48
ATOM	2318	N	PHE	294	15.022	20.317	38.058	1.00	13.04
ATOM	2319	CA	PHE	294	15.077	18.880	38.281	1.00	12.53
ATOM	2320	CB	PHE	294	14.088	18.492	39.388	1.00	11.94
ATOM	2321	CG	PHE	294	14.388	19.125	40.730	1.00	12.10
ATOM	2322	CD1	PHE	294	13.528	18.944	41.806	1.00	11.69
ATOM	2323	CD2	PHE	294	15.537	19.896	40.920	1.00	13.38
ATOM	2324	CE1	PHE	294	13.801	19.516	43.064	1.00	13.21
ATOM	2325	CE2	PHE	294	15.819	20.472	42.164	1.00	14.60
ATOM	2326	CZ	PHE	294	14.950	20.282	43.238	1.00	13.81
ATOM	2327	C	PHE	294	14.833	18.071	37.009	1.00	12.33
ATOM	2328	O	PHE	294	15.485	17.063	36.783	1.00	12.23
ATOM	2329	N	ALA	295	13.896	18.515	36.174	1.00	12.05
ATOM	2330	CA	ALA	295	13.614	17.831	34.915	1.00	12.62
ATOM	2331	CB	ALA	295	12.438	18.521	34.195	1.00	12.65
ATOM	2332	C	ALA	295	14.868	17.870	34.030	1.00	13.64
ATOM	2333	O	ALA	295	15.275	16.864	33.449	1.00	12.58
ATOM	2334	N	LYS	296	15.474	19.046	33.925	1.00	14.35
ATOM	2335	CA	LYS	296	16.681	19.214	33.129	1.00	15.93
ATOM	2336	CB	LYS	296	17.120	20.685	33.183	1.00	19.49
ATOM	2337	CG	LYS	296	18.232	21.045	32.236	1.00	23.36
ATOM	2338	CD	LYS	296	18.995	22.281	32.700	1.00	26.51
ATOM	2339	CE	LYS	296	20.353	22.337	32.030	1.00	28.90
ATOM	2340	NZ	LYS	296	21.367	23.121	32.804	1.00	31.60
ATOM	2341	C	LYS	296	17.799	18.291	33.643	1.00	15.26
ATOM	2342	O	LYS	296	18.476	17.629	32.852	1.00	15.35
ATOM	2343	N	ALA	297	17.973	18.230	34.964	1.00	14.59
ATOM	2344	CA	ALA	297	19.008	17.398	35.586	1.00	13.50
ATOM	2345	CB	ALA	297	19.010	17.608	37.093	1.00	13.72
ATOM	2346	C	ALA	297	18.855	15.914	35.300	1.00	13.36
ATOM	2347	O	ALA	297	19.846	15.183	35.243	1.00	13.45
ATOM	2348	N	LEU	298	17.613	15.458	35.157	1.00	12.73
ATOM	2349	CA	LEU	298	17.374	14.047	34.903	1.00	12.91
ATOM	2350	CB	LEU	298	16.272	13.525	35.829	1.00	13.32
ATOM	2351	CG	LEU	298	16.593	13.731	37.320	1.00	14.27
ATOM	2352	CD1	LEU	298	15.449	13.229	38.186	1.00	15.36

ATOM	2353	CD2	LEU	298	17.886	13.014	37.665	1.00	13.89
ATOM	2354	C	LEU	298	17.044	13.766	33.442	1.00	13.41
ATOM	2355	O	LEU	298	16.722	12.630	33.067	1.00	13.84
ATOM	2356	N	GLY	299	17.126	14.804	32.620	1.00	12.79
ATOM	2357	CA	GLY	299	16.883	14.648	31.194	1.00	13.44
ATOM	2358	C	GLY	299	15.450	14.424	30.754	1.00	13.52
ATOM	2359	O	GLY	299	15.214	13.800	29.721	1.00	12.79
ATOM	2360	N	VAL	300	14.513	14.937	31.545	1.00	13.04
ATOM	2361	CA	VAL	300	13.076	14.856	31.304	1.00	13.70
ATOM	2362	CB	VAL	300	12.315	14.879	32.665	1.00	15.17
ATOM	2363	CG1	VAL	300	10.822	14.786	32.456	1.00	17.34
ATOM	2364	CG2	VAL	300	12.800	13.758	33.547	1.00	16.74
ATOM	2365	C	VAL	300	12.658	16.107	30.524	1.00	13.86
ATOM	2366	O	VAL	300	13.269	17.159	30.691	1.00	11.52
ATOM	2367	N	MET	301	11.621	16.005	29.693	1.00	14.27
ATOM	2368	CA	MET	301	11.139	17.174	28.958	1.00	15.70
ATOM	2369	CB	MET	301	9.958	16.802	28.061	1.00	18.79
ATOM	2370	CG	MET	301	10.332	15.838	26.940	1.00	22.01
ATOM	2371	SD	MET	301	9.434	16.143	25.435	1.00	26.15
ATOM	2372	CE	MET	301	8.117	15.221	25.615	1.00	27.39
ATOM	2373	C	MET	301	10.728	18.222	29.990	1.00	15.78
ATOM	2374	O	MET	301	9.954	17.926	30.907	1.00	14.80
ATOM	2375	N	ASP	302	11.244	19.444	29.857	1.00	16.88
ATOM	2376	CA	ASP	302	10.952	20.479	30.840	1.00	17.75
ATOM	2377	CB	ASP	302	12.267	21.077	31.366	1.00	19.75
ATOM	2378	CG	ASP	302	13.119	21.705	30.267	1.00	21.85
ATOM	2379	OD1	ASP	302	12.737	21.619	29.078	1.00	23.40
ATOM	2380	OD2	ASP	302	14.187	22.283	30.598	1.00	22.38
ATOM	2381	C	ASP	302	10.004	21.601	30.433	1.00	17.07
ATOM	2382	O	ASP	302	9.787	22.541	31.202	1.00	18.55
ATOM	2383	N	ASP	303	9.420	21.524	29.248	1.00	15.32
ATOM	2384	CA	ASP	303	8.506	22.592	28.863	1.00	14.89
ATOM	2385	CB	ASP	303	8.534	22.812	27.343	1.00	16.89
ATOM	2386	CG	ASP	303	7.958	21.651	26.580	1.00	18.41
ATOM	2387	OD1	ASP	303	8.498	20.532	26.726	1.00	18.09
ATOM	2388	OD2	ASP	303	6.965	21.867	25.836	1.00	18.85
ATOM	2389	C	ASP	303	7.095	22.258	29.339	1.00	14.01
ATOM	2390	O	ASP	303	6.753	21.087	29.544	1.00	12.95
ATOM	2391	N	LEU	304	6.283	23.289	29.524	1.00	12.17
ATOM	2392	CA	LEU	304	4.919	23.091	29.999	1.00	11.78
ATOM	2393	CB	LEU	304	4.782	23.615	31.440	1.00	12.96
ATOM	2394	CG	LEU	304	5.798	23.160	32.495	1.00	13.16
ATOM	2395	CD1	LEU	304	6.721	24.315	32.846	1.00	14.56
ATOM	2396	CD2	LEU	304	5.063	22.670	33.738	1.00	14.55
ATOM	2397	C	LEU	304	3.894	23.788	29.110	1.00	11.34
ATOM	2398	O	LEU	304	4.154	24.869	28.592	1.00	11.00
ATOM	2399	N	LYS	305	2.738	23.152	28.924	1.00	10.43
ATOM	2400	CA	LYS	305	1.660	23.739	28.131	1.00	9.26
ATOM	2401	CB	LYS	305	1.240	22.794	27.010	1.00	10.66
ATOM	2402	CG	LYS	305	2.352	22.504	26.020	1.00	11.25
ATOM	2403	CD	LYS	305	2.730	23.744	25.237	1.00	14.11
ATOM	2404	CE	LYS	305	3.614	23.380	24.053	1.00	13.92
ATOM	2405	NZ	LYS	305	3.688	24.465	23.047	1.00	16.93
ATOM	2406	C	LYS	305	.505	23.971	29.091	1.00	9.24
ATOM	2407	O	LYS	305	.005	23.034	29.709	1.00	9.35
ATOM	2408	N	SER	306	.101	25.231	29.229	1.00	7.91
ATOM	2409	CA	SER	306	-.972	25.607	30.143	1.00	8.70
ATOM	2410	CB	SER	306	-2.327	25.079	29.667	1.00	8.96
ATOM	2411	OG	SER	306	-2.737	25.715	28.472	1.00	9.50
ATOM	2412	C	SER	306	-.660	25.079	31.541	1.00	8.78

ATOM	2413	O	SER	306	-1.553	24.674	32.290	1.00	8.31
ATOM	2414	N	GLY	307	.631	25.069	31.868	1.00	8.91
ATOM	2415	CA	GLY	307	1.074	24.636	33.179	1.00	8.81
ATOM	2416	C	GLY	307	1.228	23.147	33.364	1.00	8.14
ATOM	2417	O	GLY	307	1.584	22.696	34.451	1.00	9.05
ATOM	2418	N	VAL	308	.995	22.373	32.305	1.00	7.83
ATOM	2419	CA	VAL	308	1.092	20.919	32.411	1.00	8.01
ATOM	2420	CB	VAL	308	-.094	20.218	31.667	1.00	7.16
ATOM	2421	CG1	VAL	308	-.064	18.719	31.935	1.00	8.25
ATOM	2422	CG2	VAL	308	-1.435	20.805	32.121	1.00	8.28
ATOM	2423	C	VAL	308	2.410	20.386	31.856	1.00	7.96
ATOM	2424	O	VAL	308	2.810	20.724	30.740	1.00	7.81
ATOM	2425	N	PRO	309	3.131	19.576	32.648	1.00	8.75
ATOM	2426	CD	PRO	309	2.984	19.228	34.075	1.00	9.93
ATOM	2427	CA	PRO	309	4.387	19.065	32.094	1.00	8.23
ATOM	2428	CB	PRO	309	5.176	18.628	33.337	1.00	9.77
ATOM	2429	CG	PRO	309	4.137	18.239	34.303	1.00	10.31
ATOM	2430	C	PRO	309	4.109	17.910	31.136	1.00	8.50
ATOM	2431	O	PRO	309	3.045	17.305	31.182	1.00	7.71
ATOM	2432	N	ARG	310	5.064	17.630	30.259	1.00	8.33
ATOM	2433	CA	ARG	310	4.920	16.520	29.314	1.00	9.66
ATOM	2434	CB	ARG	310	6.167	16.430	28.449	1.00	12.40
ATOM	2435	CG	ARG	310	6.492	17.715	27.737	1.00	16.98
ATOM	2436	CD	ARG	310	5.901	17.695	26.365	1.00	19.23
ATOM	2437	NE	ARG	310	6.157	18.947	25.663	1.00	22.12
ATOM	2438	CZ	ARG	310	5.838	19.138	24.395	1.00	23.16
ATOM	2439	NH1	ARG	310	5.267	18.147	23.715	1.00	24.77
ATOM	2440	NH2	ARG	310	6.059	20.319	23.828	1.00	24.54
ATOM	2441	C	ARG	310	4.747	15.221	30.098	1.00	8.87
ATOM	2442	O	ARG	310	5.488	14.959	31.055	1.00	9.01
ATOM	2443	N	ALA	311	3.779	14.414	29.673	1.00	9.24
ATOM	2444	CA	ALA	311	3.444	13.129	30.311	1.00	9.88
ATOM	2445	CB	ALA	311	4.613	12.136	30.177	1.00	10.38
ATOM	2446	C	ALA	311	3.037	13.236	31.776	1.00	9.03
ATOM	2447	O	ALA	311	2.903	12.218	32.474	1.00	9.95
ATOM	2448	N	GLY	312	2.813	14.451	32.250	1.00	8.54
ATOM	2449	CA	GLY	312	2.448	14.617	33.644	1.00	7.93
ATOM	2450	C	GLY	312	1.036	14.208	34.012	1.00	7.04
ATOM	2451	O	GLY	312	.134	14.282	33.190	1.00	7.03
ATOM	2452	N	TYR	313	.854	13.740	35.245	1.00	5.72
ATOM	2453	CA	TYR	313	-.463	13.370	35.749	1.00	5.61
ATOM	2454	CB	TYR	313	-.680	11.859	35.697	1.00	6.39
ATOM	2455	CG	TYR	313	-2.102	11.488	36.043	1.00	7.06
ATOM	2456	CD1	TYR	313	-3.156	11.865	35.214	1.00	8.05
ATOM	2457	CE1	TYR	313	-4.471	11.578	35.548	1.00	9.00
ATOM	2458	CD2	TYR	313	-2.399	10.813	37.220	1.00	7.11
ATOM	2459	CE2	TYR	313	-3.712	10.528	37.569	1.00	8.51
ATOM	2460	CZ	TYR	313	-4.739	10.908	36.731	1.00	8.41
ATOM	2461	OH	TYR	313	-6.036	10.593	37.066	1.00	11.71
ATOM	2462	C	TYR	313	-.500	13.865	37.192	1.00	7.11
ATOM	2463	O	TYR	313	.282	13.413	38.026	1.00	8.07
ATOM	2464	N	ARG	314	-1.410	14.795	37.475	1.00	7.02
ATOM	2465	CA	ARG	314	-1.497	15.408	38.800	1.00	7.66
ATOM	2466	CB	ARG	314	-1.991	14.393	39.846	1.00	7.96
ATOM	2467	CG	ARG	314	-3.438	13.922	39.608	1.00	9.34
ATOM	2468	CD	ARG	314	-4.030	13.170	40.818	1.00	11.37
ATOM	2469	NE	ARG	314	-4.194	14.036	41.993	1.00	13.36
ATOM	2470	CZ	ARG	314	-5.262	14.804	42.220	1.00	14.20
ATOM	2471	NH1	ARG	314	-6.276	14.817	41.359	1.00	15.56
ATOM	2472	NH2	ARG	314	-5.322	15.566	43.312	1.00	16.32

ATOM	2473	C	ARG	314	-.104	15.948	39.143	1.00	7.77
ATOM	2474	O	ARG	314	.369	15.852	40.281	1.00	8.07
ATOM	2475	N	GLY	315	.540	16.511	38.117	1.00	6.58
ATOM	2476	CA	GLY	315	1.875	17.083	38.238	1.00	7.53
ATOM	2477	C	GLY	315	3.042	16.110	38.268	1.00	7.50
ATOM	2478	O	GLY	315	4.209	16.516	38.269	1.00	7.44
ATOM	2479	N	ILE	316	2.732	14.818	38.236	1.00	7.11
ATOM	2480	CA	ILE	316	3.747	13.788	38.317	1.00	7.57
ATOM	2481	CB	ILE	316	3.215	12.571	39.107	1.00	8.57
ATOM	2482	CG2	ILE	316	4.338	11.566	39.342	1.00	7.35
ATOM	2483	CG1	ILE	316	2.594	13.041	40.425	1.00	9.70
ATOM	2484	CD1	ILE	316	1.736	12.006	41.098	1.00	11.43
ATOM	2485	C	ILE	316	4.221	13.284	36.962	1.00	7.50
ATOM	2486	O	ILE	316	3.412	12.871	36.138	1.00	7.21
ATOM	2487	N	VAL	317	5.533	13.335	36.748	1.00	7.72
ATOM	2488	CA	VAL	317	6.150	12.843	35.522	1.00	7.80
ATOM	2489	CB	VAL	317	7.150	13.854	34.947	1.00	6.78
ATOM	2490	CG1	VAL	317	7.708	13.342	33.630	1.00	7.94
ATOM	2491	CG2	VAL	317	6.462	15.204	34.747	1.00	7.41
ATOM	2492	C	VAL	317	6.875	11.551	35.913	1.00	7.41
ATOM	2493	O	VAL	317	7.751	11.553	36.785	1.00	7.43
ATOM	2494	N	THR	318	6.497	10.447	35.274	1.00	7.68
ATOM	2495	CA	THR	318	7.057	9.128	35.586	1.00	7.76
ATOM	2496	CB	THR	318	5.914	8.128	35.882	1.00	7.45
ATOM	2497	OG1	THR	318	5.153	8.605	37.001	1.00	8.76
ATOM	2498	CG2	THR	318	6.468	6.726	36.201	1.00	9.39
ATOM	2499	C	THR	318	7.923	8.612	34.445	1.00	8.03
ATOM	2500	O	THR	318	7.510	8.629	33.301	1.00	8.87
ATOM	2501	N	PHE	319	9.117	8.134	34.784	1.00	8.14
ATOM	2502	CA	PHE	319	10.068	7.668	33.783	1.00	8.19
ATOM	2503	CB	PHE	319	10.776	8.897	33.171	1.00	8.94
ATOM	2504	CG	PHE	319	11.433	9.801	34.196	1.00	9.51
ATOM	2505	CD1	PHE	319	12.809	9.748	34.423	1.00	10.13
ATOM	2506	CD2	PHE	319	10.670	10.701	34.949	1.00	10.78
ATOM	2507	CE1	PHE	319	13.413	10.573	35.385	1.00	9.35
ATOM	2508	CE2	PHE	319	11.269	11.524	35.908	1.00	10.62
ATOM	2509	CZ	PHE	319	12.636	11.460	36.128	1.00	10.85
ATOM	2510	C	PHE	319	11.108	6.746	34.397	1.00	9.45
ATOM	2511	O	PHE	319	11.136	6.550	35.615	1.00	8.99
ATOM	2512	N	LEU	320	11.959	6.177	33.549	1.00	11.01
ATOM	2513	CA	LEU	320	13.040	5.326	34.040	1.00	12.08
ATOM	2514	CB	LEU	320	13.158	4.027	33.217	1.00	12.46
ATOM	2515	CG	LEU	320	13.518	2.776	34.033	1.00	14.09
ATOM	2516	CD1	LEU	320	12.368	2.444	34.987	1.00	13.26
ATOM	2517	CD2	LEU	320	13.804	1.599	33.120	1.00	15.40
ATOM	2518	C	LEU	320	14.323	6.157	33.924	1.00	12.41
ATOM	2519	O	LEU	320	14.493	6.928	32.970	1.00	12.24
ATOM	2520	N	PHE	321	15.200	6.037	34.914	1.00	11.91
ATOM	2521	CA	PHE	321	16.472	6.761	34.912	1.00	11.72
ATOM	2522	CB	PHE	321	16.426	7.978	35.841	1.00	12.56
ATOM	2523	CG	PHE	321	17.642	8.861	35.732	1.00	12.85
ATOM	2524	CD1	PHE	321	17.774	9.756	34.675	1.00	12.80
ATOM	2525	CD2	PHE	321	18.671	8.778	36.675	1.00	12.28
ATOM	2526	CE1	PHE	321	18.918	10.564	34.553	1.00	12.15
ATOM	2527	CE2	PHE	321	19.817	9.580	36.562	1.00	14.10
ATOM	2528	CZ	PHE	321	19.938	10.476	35.499	1.00	13.19
ATOM	2529	C	PHE	321	17.526	5.785	35.408	1.00	12.68
ATOM	2530	O	PHE	321	17.488	5.352	36.569	1.00	11.61
ATOM	2531	N	ARG	322	18.459	5.426	34.527	1.00	13.86
ATOM	2532	CA	ARG	322	19.516	4.478	34.876	1.00	14.65

ATOM	2533	CB	ARG	322	20.483	5.091	35.884	1.00	19.60
ATOM	2534	CG	ARG	322	21.375	6.177	35.335	1.00	23.38
ATOM	2535	CD	ARG	322	21.996	6.936	36.486	1.00	27.13
ATOM	2536	NE	ARG	322	23.307	7.474	36.128	1.00	30.83
ATOM	2537	CZ	ARG	322	24.419	6.744	36.015	1.00	32.74
ATOM	2538	NH1	ARG	322	24.398	5.437	36.237	1.00	33.92
ATOM	2539	NH2	ARG	322	25.562	7.331	35.678	1.00	34.41
ATOM	2540	C	ARG	322	18.930	3.203	35.471	1.00	14.41
ATOM	2541	O	ARG	322	19.414	2.697	36.486	1.00	12.80
ATOM	2542	N	GLY	323	17.872	2.701	34.842	1.00	14.14
ATOM	2543	CA	GLY	323	17.247	1.472	35.289	1.00	14.65
ATOM	2544	C	GLY	323	16.301	1.588	36.461	1.00	15.10
ATOM	2545	O	GLY	323	15.673	.608	36.842	1.00	16.27
ATOM	2546	N	ARG	324	16.197	2.780	37.025	1.00	14.24
ATOM	2547	CA	ARG	324	15.351	3.024	38.176	1.00	15.14
ATOM	2548	CB	ARG	324	16.165	3.779	39.232	1.00	16.63
ATOM	2549	CG	ARG	324	15.327	4.629	40.143	1.00	18.62
ATOM	2550	CD	ARG	324	15.995	4.802	41.470	1.00	19.33
ATOM	2551	NE	ARG	324	17.310	5.423	41.375	1.00	17.58
ATOM	2552	CZ	ARG	324	18.161	5.486	42.393	1.00	17.19
ATOM	2553	NH1	ARG	324	17.827	4.963	43.560	1.00	16.46
ATOM	2554	NH2	ARG	324	19.340	6.070	42.251	1.00	18.03
ATOM	2555	C	ARG	324	14.068	3.791	37.850	1.00	14.04
ATOM	2556	O	ARG	324	14.086	4.727	37.047	1.00	14.16
ATOM	2557	N	ARG	325	12.956	3.383	38.461	1.00	12.09
ATOM	2558	CA	ARG	325	11.682	4.069	38.257	1.00	10.86
ATOM	2559	CB	ARG	325	10.516	3.180	38.711	1.00	10.30
ATOM	2560	CG	ARG	325	9.136	3.855	38.642	1.00	9.96
ATOM	2561	CD	ARG	325	8.772	4.223	37.207	1.00	9.56
ATOM	2562	NE	ARG	325	8.668	3.045	36.355	1.00	8.33
ATOM	2563	CZ	ARG	325	8.763	3.073	35.029	1.00	8.06
ATOM	2564	NH1	ARG	325	8.971	4.226	34.395	1.00	9.39
ATOM	2565	NH2	ARG	325	8.648	1.947	34.339	1.00	9.05
ATOM	2566	C	ARG	325	11.701	5.350	39.093	1.00	11.09
ATOM	2567	O	ARG	325	11.922	5.296	40.306	1.00	10.54
ATOM	2568	N	VAL	326	11.466	6.496	38.457	1.00	8.93
ATOM	2569	CA	VAL	326	11.463	7.781	39.161	1.00	9.45
ATOM	2570	CB	VAL	326	12.590	8.713	38.662	1.00	9.23
ATOM	2571	CG1	VAL	326	12.588	10.015	39.484	1.00	10.38
ATOM	2572	CG2	VAL	326	13.941	8.008	38.744	1.00	10.23
ATOM	2573	C	VAL	326	10.156	8.531	38.918	1.00	9.33
ATOM	2574	O	VAL	326	9.647	8.555	37.796	1.00	9.75
ATOM	2575	N	HIS	327	9.620	9.144	39.969	1.00	9.32
ATOM	2576	CA	HIS	327	8.407	9.939	39.854	1.00	8.60
ATOM	2577	CB	HIS	327	7.336	9.423	40.811	1.00	8.98
ATOM	2578	CG	HIS	327	6.960	7.996	40.585	1.00	9.12
ATOM	2579	CD2	HIS	327	7.147	6.896	41.352	1.00	10.26
ATOM	2580	ND1	HIS	327	6.301	7.565	39.451	1.00	9.71
ATOM	2581	CE1	HIS	327	6.093	6.261	39.534	1.00	9.28
ATOM	2582	NE2	HIS	327	6.598	5.832	40.679	1.00	10.29
ATOM	2583	C	HIS	327	8.789	11.368	40.250	1.00	9.37
ATOM	2584	O	HIS	327	9.088	11.624	41.418	1.00	9.76
ATOM	2585	N	LEU	328	8.800	12.283	39.286	1.00	8.47
ATOM	2586	CA	LEU	328	9.114	13.688	39.562	1.00	9.22
ATOM	2587	CB	LEU	328	9.696	14.346	38.308	1.00	9.12
ATOM	2588	CG	LEU	328	10.049	15.834	38.351	1.00	11.32
ATOM	2589	CD1	LEU	328	10.999	16.095	39.507	1.00	11.44
ATOM	2590	CD2	LEU	328	10.670	16.257	37.014	1.00	11.07
ATOM	2591	C	LEU	328	7.740	14.233	39.938	1.00	9.98
ATOM	2592	O	LEU	328	6.855	14.404	39.084	1.00	10.11

ATOM	2593	N	ALA	329	7.576	14.491	41.233	1.00	9.80
ATOM	2594	CA	ALA	329	6.287	14.874	41.786	1.00	9.71
ATOM	2595	CB	ALA	329	5.739	13.691	42.577	1.00	7.90
ATOM	2596	C	ALA	329	6.199	16.099	42.652	1.00	9.26
ATOM	2597	O	ALA	329	7.161	16.507	43.294	1.00	9.87
ATOM	2598	N	PRO	330	5.012	16.704	42.690	1.00	9.84
ATOM	2599	CD	PRO	330	3.853	16.504	41.794	1.00	8.95
ATOM	2600	CA	PRO	330	4.829	17.889	43.524	1.00	10.11
ATOM	2601	CB	PRO	330	3.679	18.605	42.831	1.00	10.04
ATOM	2602	CG	PRO	330	2.809	17.446	42.380	1.00	8.88
ATOM	2603	C	PRO	330	4.428	17.368	44.907	1.00	10.96
ATOM	2604	O	PRO	330	4.302	16.156	45.119	1.00	10.01
ATOM	2605	N	PRO	331	4.224	18.270	45.866	1.00	12.09
ATOM	2606	CD	PRO	331	4.340	19.736	45.857	1.00	13.32
ATOM	2607	CA	PRO	331	3.827	17.768	47.185	1.00	13.78
ATOM	2608	CB	PRO	331	3.737	19.038	48.024	1.00	13.49
ATOM	2609	CG	PRO	331	4.627	20.021	47.305	1.00	14.64
ATOM	2610	C	PRO	331	2.451	17.144	46.968	1.00	13.55
ATOM	2611	O	PRO	331	1.746	17.561	46.055	1.00	12.81
ATOM	2612	N	GLN	332	2.045	16.182	47.793	1.00	14.71
ATOM	2613	CA	GLN	332	.741	15.560	47.565	1.00	16.10
ATOM	2614	CB	GLN	332	.575	14.247	48.348	1.00	16.78
ATOM	2615	CG	GLN	332	-.692	13.489	47.919	1.00	19.39
ATOM	2616	CD	GLN	332	-.761	12.069	48.448	1.00	19.63
ATOM	2617	OE1	GLN	332	-.025	11.702	49.372	1.00	20.06
ATOM	2618	NE2	GLN	332	-1.648	11.263	47.868	1.00	19.43
ATOM	2619	C	GLN	332	-.431	16.493	47.860	1.00	16.64
ATOM	2620	O	GLN	332	-1.586	16.084	47.795	1.00	17.44
ATOM	2621	N	THR	333	-.137	17.748	48.180	1.00	17.06
ATOM	2622	CA	THR	333	-1.185	18.733	48.411	1.00	17.47
ATOM	2623	CB	THR	333	-.689	19.864	49.322	1.00	17.84
ATOM	2624	OG1	THR	333	.653	20.215	48.959	1.00	18.71
ATOM	2625	CG2	THR	333	-.732	19.420	50.783	1.00	18.81
ATOM	2626	C	THR	333	-1.605	19.342	47.068	1.00	16.99
ATOM	2627	O	THR	333	-2.498	20.195	47.016	1.00	17.43
ATOM	2628	N	TRP	334	-.936	18.911	45.997	1.00	15.05
ATOM	2629	CA	TRP	334	-1.218	19.388	44.646	1.00	15.42
ATOM	2630	CB	TRP	334	-.529	18.493	43.611	1.00	13.12
ATOM	2631	CG	TRP	334	-.693	18.946	42.177	1.00	12.68
ATOM	2632	CD2	TRP	334	-1.769	18.616	41.291	1.00	11.70
ATOM	2633	CE2	TRP	334	-1.505	19.254	40.056	1.00	10.82
ATOM	2634	CE3	TRP	334	-2.931	17.846	41.421	1.00	11.17
ATOM	2635	CD1	TRP	334	.155	19.750	41.467	1.00	11.49
ATOM	2636	NE1	TRP	334	-.323	19.940	40.191	1.00	11.34
ATOM	2637	CZ2	TRP	334	-2.361	19.140	38.960	1.00	10.22
ATOM	2638	CZ3	TRP	334	-3.786	17.733	40.330	1.00	11.42
ATOM	2639	CH2	TRP	334	-3.492	18.382	39.110	1.00	11.18
ATOM	2640	C	TRP	334	-2.722	19.359	44.402	1.00	15.81
ATOM	2641	O	TRP	334	-3.399	18.389	44.748	1.00	16.58
ATOM	2642	N	ASP	335	-3.239	20.409	43.772	1.00	17.32
ATOM	2643	CA	ASP	335	-4.663	20.485	43.487	1.00	18.28
ATOM	2644	CB	ASP	335	-5.397	21.025	44.717	1.00	22.00
ATOM	2645	CG	ASP	335	-6.901	21.062	44.526	1.00	24.35
ATOM	2646	OD1	ASP	335	-7.563	21.898	45.189	1.00	26.10
ATOM	2647	OD2	ASP	335	-7.418	20.253	43.715	1.00	25.60
ATOM	2648	C	ASP	335	-4.989	21.346	42.260	1.00	18.45
ATOM	2649	O	ASP	335	-5.714	22.331	42.353	1.00	19.37
ATOM	2650	N	GLY	336	-4.470	20.957	41.098	1.00	16.45
ATOM	2651	CA	GLY	336	-4.755	21.708	39.892	1.00	14.26
ATOM	2652	C	GLY	336	-3.526	22.345	39.284	1.00	13.54

ATOM	2653	O	GLY	336	-2.537	22.602	39.970	1.00 13.72	
ATOM	2654	N	TYR	337	-3.582	22.586	37.983	1.00 12.73	
ATOM	2655	CA	TYR	337	-2.469	23.197	37.283	1.00 12.09	
ATOM	2656	CB	TYR	337	-2.366	22.639	35.863	1.00 10.35	
ATOM	2657	CG	TYR	337	-2.010	21.183	35.820	1.00 8.81	
ATOM	2658	CD1	TYR	337	-2.986	20.209	35.594	1.00 8.57	
ATOM	2659	CE1	TYR	337	-2.650	18.862	35.540	1.00 7.63	
ATOM	2660	CD2	TYR	337	-.682	20.772	35.995	1.00 9.04	
ATOM	2661	CE2	TYR	337	-.339	19.443	35.940	1.00 9.03	
ATOM	2662	CZ	TYR	337	-1.316	18.486	35.711	1.00 9.43	
ATOM	2663	OH	TYR	337	-.941	17.165	35.651	1.00 8.82	
ATOM	2664	C	TYR	337	-2.551	24.721	37.206	1.00 12.72	
ATOM	2665	O	TYR	337	-3.631	25.298	37.090	1.00 12.92	
ATOM	2666	N	ASP	338	-1.389	25.357	37.282	1.00 11.77	
ATOM	2667	CA	ASP	338	-1.281	26.818	37.205	1.00 12.54	
ATOM	2668	CB	ASP	338	-.324	27.305	38.300	1.00 14.69	
ATOM	2669	CG	ASP	338	-.212	28.816	38.366	1.00 16.42	
ATOM	2670	OD1	ASP	338	-.690	29.487	37.431	1.00 17.17	
ATOM	2671	OD2	ASP	338	.376	29.323	39.354	1.00 17.95	
ATOM	2672	C	ASP	338	-.727	27.152	35.812	1.00 11.95	
ATOM	2673	O	ASP	338	.419	26.855	35.517	1.00 10.52	
ATOM	2674	N	PRO	339	-1.537	27.772	34.940	1.00 11.90	
ATOM	2675	CD	PRO	339	-2.979	28.038	35.051	1.00 13.16	
ATOM	2676	CA	PRO	339	-1.058	28.107	33.594	1.00 11.72	
ATOM	2677	CB	PRO	339	-2.298	28.685	32.915	1.00 13.77	
ATOM	2678	CG	PRO	339	-3.407	27.983	33.596	1.00 15.25	
ATOM	2679	C	PRO	339	.115	29.077	33.556	1.00 11.13	
ATOM	2680	O	PRO	339	.776	29.180	32.530	1.00 10.92	
ATOM	2681	N	SER	340	.378	29.785	34.656	1.00 10.66	
ATOM	2682	CA	SER	340	1.490	30.735	34.680	1.00 11.33	
ATOM	2683	CB	SER	340	1.380	31.693	35.868	1.00 11.99	
ATOM	2684	OG	SER	340	1.790	31.086	37.078	1.00 15.02	
ATOM	2685	C	SER	340	2.843	30.045	34.727	1.00 11.74	
ATOM	2686	O	SER	340	3.889	30.702	34.621	1.00 11.68	
ATOM	2687	N	TRP	341	2.822	28.727	34.933	1.00 11.17	
ATOM	2688	CA	TRP	341	4.055	27.939	34.938	1.00 11.32	
ATOM	2689	CB	TRP	341	3.821	26.565	35.565	1.00 11.63	
ATOM	2690	CG	TRP	341	3.824	26.578	37.060	1.00 11.35	
ATOM	2691	CD2	TRP	341	4.398	25.585	37.914	1.00 12.13	
ATOM	2692	CE2	TRP	341	4.119	25.964	39.244	1.00 12.04	
ATOM	2693	CE3	TRP	341	5.126	24.407	37.683	1.00 12.44	
ATOM	2694	CD1	TRP	341	3.235	27.500	37.883	1.00 11.81	
ATOM	2695	NE1	TRP	341	3.411	27.138	39.197	1.00 12.20	
ATOM	2696	CZ2	TRP	341	4.539	25.205	40.343	1.00 13.56	
ATOM	2697	CZ3	TRP	341	5.547	23.653	38.773	1.00 12.86	
ATOM	2698	CH2	TRP	341	5.252	24.054	40.085	1.00 12.69	
ATOM	2699	C	TRP	341	4.382	27.775	33.468	1.00 10.74	
ATOM	2700	O	TRP	341	3.876	26.870	32.804	1.00 10.69	
ATOM	2701	N	THR	342	5.224	28.669	32.963	1.00 11.51	
ATOM	2702	CA	THR	342	5.587	28.663	31.565	1.00 12.93	
ATOM	2703	CB	THR	342	5.271	30.029	30.940	1.00 12.14	
ATOM	2704	OG1	THR	342	5.966	31.047	31.673	1.00 11.94	
ATOM	2705	CG2	THR	342	3.769	30.292	30.975	1.00 12.23	
ATOM	2706	C	THR	342	7.062	28.344	31.322	1.00 14.68	
ATOM	2707	O	THR	342	7.508	28.352	30.162	1.00 15.15	
ATOM	2708	HG	MMC	1268	.888	6.652	9.745	1.00 2.00	
ATOM	2709	C	MMC	1268	.788	6.090	11.659	1.00 8.03	
ATOM	2710	OH2	TIP	1	.227	8.802	35.495	1.00 8.47	S
ATOM	2711	OH2	TIP	2	-2.594	14.784	15.457	1.00 10.01	S
ATOM	2712	OH2	TIP	3	-1.705	-4.084	16.155	1.00 7.25	S

ATOM	2713	OH2 TIP	4	2.604	26.646	30.390	1.00 14.12	S
ATOM	2714	OH2 TIP	5	2.968	10.081	36.301	1.00 11.23	S
ATOM	2715	OH2 TIP	6	3.318	35.567	17.089	1.00 11.53	S
ATOM	2716	OH2 TIP	7	-5.301	21.950	30.553	1.00 12.15	S
ATOM	2717	OH2 TIP	8	5.371	-6.955	36.149	1.00 11.67	S
ATOM	2718	OH2 TIP	9	-3.183	18.558	27.781	1.00 10.51	S
ATOM	2719	OH2 TIP	10	-2.593	24.445	13.661	1.00 12.07	S
ATOM	2720	OH2 TIP	11	-5.293	15.356	28.445	1.00 11.61	S
ATOM	2721	OH2 TIP	12	-12.760	11.329	22.960	1.00 8.77	S
ATOM	2722	OH2 TIP	13	-6.023	23.491	4.761	1.00 10.83	S
ATOM	2723	OH2 TIP	14	4.160	-11.017	21.146	1.00 17.57	S
ATOM	2724	OH2 TIP	15	.167	15.364	16.847	1.00 14.09	S
ATOM	2725	OH2 TIP	16	1.488	9.838	32.116	1.00 8.29	S
ATOM	2726	OH2 TIP	17	-1.332	11.930	15.068	1.00 12.12	S
ATOM	2727	OH2 TIP	18	-1.752	-2.886	30.502	1.00 12.96	S
ATOM	2728	OH2 TIP	19	-1.623	25.054	25.975	1.00 9.70	S
ATOM	2729	OH2 TIP	20	-9.234	.870	4.261	1.00 8.84	S
ATOM	2730	OH2 TIP	21	-6.357	-4.248	36.027	1.00 13.00	S
ATOM	2731	OH2 TIP	22	3.924	.287	27.226	1.00 10.49	S
ATOM	2732	OH2 TIP	23	3.167	10.752	26.936	1.00 10.35	S
ATOM	2733	OH2 TIP	24	5.383	3.493	36.814	1.00 15.04	S
ATOM	2734	OH2 TIP	25	3.409	15.422	22.360	1.00 16.92	S
ATOM	2735	OH2 TIP	26	-15.687	18.469	6.443	1.00 17.60	S
ATOM	2736	OH2 TIP	27	1.024	35.621	19.225	1.00 14.07	S
ATOM	2737	OH2 TIP	28	-1.313	-14.037	23.809	1.00 14.97	S
ATOM	2738	OH2 TIP	29	.938	-7.089	14.209	1.00 12.96	S
ATOM	2739	OH2 TIP	30	-2.230	29.263	25.256	1.00 21.69	S
ATOM	2740	OH2 TIP	31	-14.648	9.593	27.344	1.00 12.59	S
ATOM	2741	OH2 TIP	32	.147	14.905	42.851	1.00 11.29	S
ATOM	2742	OH2 TIP	33	-14.449	11.610	25.304	1.00 17.71	S
ATOM	2743	OH2 TIP	34	-4.716	-7.984	16.971	1.00 12.05	S
ATOM	2744	OH2 TIP	35	6.648	6.129	31.616	1.00 11.76	S
ATOM	2745	OH2 TIP	36	4.551	36.162	12.621	1.00 17.93	S
ATOM	2746	OH2 TIP	37	-19.337	14.462	15.904	1.00 17.84	S
ATOM	2747	OH2 TIP	38	-7.488	28.123	9.804	1.00 16.87	S
ATOM	2748	OH2 TIP	39	7.131	10.062	30.808	1.00 13.25	S
ATOM	2749	OH2 TIP	40	-5.994	21.922	36.510	1.00 14.05	S
ATOM	2750	OH2 TIP	41	.467	32.931	18.689	1.00 18.58	S
ATOM	2751	OH2 TIP	42	3.763	21.864	-1.616	1.00 22.14	S
ATOM	2752	OH2 TIP	43	7.868	25.759	29.234	1.00 11.72	S
ATOM	2753	OH2 TIP	44	-8.338	-5.706	27.382	1.00 17.04	S
ATOM	2754	OH2 TIP	45	-1.846	21.178	28.892	1.00 11.34	S
ATOM	2755	OH2 TIP	46	-4.509	1.856	38.991	1.00 20.30	S
ATOM	2756	OH2 TIP	47	-4.127	23.916	32.475	1.00 14.11	S
ATOM	2757	OH2 TIP	48	-3.457	-6.171	15.064	1.00 10.57	S
ATOM	2758	OH2 TIP	49	-2.202	28.384	28.339	1.00 17.90	S
ATOM	2759	OH2 TIP	50	-7.077	42.084	13.485	1.00 18.59	S
ATOM	2760	OH2 TIP	51	7.472	18.942	31.067	1.00 11.41	S
ATOM	2761	OH2 TIP	52	-8.191	21.373	32.070	1.00 15.67	S
ATOM	2762	OH2 TIP	53	9.257	7.626	30.295	1.00 12.02	S
ATOM	2763	OH2 TIP	54	8.188	15.590	31.124	1.00 10.90	S
ATOM	2764	OH2 TIP	55	-13.611	21.454	25.053	1.00 16.25	S
ATOM	2765	OH2 TIP	56	10.078	-5.295	24.969	1.00 17.41	S
ATOM	2766	OH2 TIP	57	-1.764	22.739	42.783	1.00 16.62	S
ATOM	2767	OH2 TIP	58	-11.438	3.221	3.824	1.00 17.91	S
ATOM	2768	OH2 TIP	59	-5.648	21.986	33.849	1.00 16.92	S
ATOM	2769	OH2 TIP	60	4.264	10.136	33.596	1.00 15.92	S
ATOM	2770	OH2 TIP	61	.224	28.873	29.842	1.00 12.74	S
ATOM	2771	OH2 TIP	62	2.829	38.795	12.374	1.00 15.52	S
ATOM	2772	OH2 TIP	63	2.037	13.645	2.488	1.00 13.47	S

ATOM	2773	OH2	TIP	64	-9.216	28.820	24.545	1.00	15.35	S
ATOM	2774	OH2	TIP	65	8.416	6.335	1.560	1.00	20.80	S
ATOM	2775	OH2	TIP	66	-9.489	26.199	11.468	1.00	18.11	S
ATOM	2776	OH2	TIP	67	9.536	4.878	31.831	1.00	17.68	S
ATOM	2777	OH2	TIP	68	8.733	5.044	23.692	1.00	13.03	S
ATOM	2778	OH2	TIP	69	2.031	-2.881	3.366	1.00	16.21	S
ATOM	2779	OH2	TIP	70	-18.818	9.137	20.239	1.00	25.43	S
ATOM	2780	OH2	TIP	71	19.256	6.748	39.424	1.00	20.75	S
ATOM	2781	OH2	TIP	72	-12.399	14.042	-2.151	1.00	23.07	S
ATOM	2782	OH2	TIP	73	2.631	3.864	9.956	1.00	15.32	S
ATOM	2783	OH2	TIP	75	-9.244	40.705	15.547	1.00	20.70	S
ATOM	2784	OH2	TIP	76	-1.187	31.698	23.028	1.00	21.29	S
ATOM	2785	OH2	TIP	77	-.342	22.625	14.393	1.00	19.99	S
ATOM	2786	OH2	TIP	78	-5.142	17.773	-1.880	1.00	17.84	S
ATOM	2787	OH2	TIP	79	1.144	23.962	37.083	1.00	21.05	S
ATOM	2788	OH2	TIP	80	6.460	7.581	-2.039	1.00	16.23	S
ATOM	2789	OH2	TIP	81	1.939	13.449	27.710	1.00	18.19	S
ATOM	2790	OH2	TIP	82	-8.963	31.014	16.937	1.00	17.18	S
ATOM	2791	OH2	TIP	83	4.951	.918	-1.187	1.00	19.02	S
ATOM	2792	OH2	TIP	84	-12.298	23.343	4.127	1.00	16.18	S
ATOM	2793	OH2	TIP	85	15.545	6.233	22.069	1.00	25.86	S
ATOM	2794	OH2	TIP	86	-4.871	-.570	40.357	1.00	17.57	S
ATOM	2795	OH2	TIP	87	-10.243	3.686	-2.697	1.00	21.88	S
ATOM	2796	OH2	TIP	88	13.191	15.201	46.459	1.00	14.10	S
ATOM	2797	OH2	TIP	89	6.269	-7.698	31.848	1.00	14.20	S
ATOM	2798	OH2	TIP	90	17.048	-1.959	42.858	1.00	22.15	S
ATOM	2799	OH2	TIP	91	-4.191	-4.208	5.622	1.00	22.19	S
ATOM	2800	OH2	TIP	92	3.515	32.191	6.887	1.00	18.38	S
ATOM	2801	OH2	TIP	93	9.519	-2.838	23.232	1.00	23.76	S
ATOM	2802	OH2	TIP	94	5.638	2.734	46.633	1.00	21.05	S
ATOM	2803	OH2	TIP	95	-10.495	-3.962	26.723	1.00	19.15	S
ATOM	2804	OH2	TIP	96	20.448	4.378	31.421	1.00	17.26	S
ATOM	2805	OH2	TIP	97	1.990	19.159	-7.451	1.00	19.66	S
ATOM	2806	OH2	TIP	98	-5.600	-4.144	2.694	1.00	22.57	S
ATOM	2807	OH2	TIP	99	-4.293	7.153	47.409	1.00	20.60	S
ATOM	2808	OH2	TIP	100	-6.354	5.000	-2.941	1.00	13.28	S
ATOM	2809	OH2	TIP	101	-.448	19.331	13.654	1.00	22.63	S
ATOM	2810	OH2	TIP	102	-1.904	21.847	5.605	1.00	26.04	S
ATOM	2811	OH2	TIP	103	-17.479	9.915	27.638	1.00	19.49	S
ATOM	2812	OH2	TIP	104	-8.020	11.975	35.486	1.00	18.42	S
ATOM	2813	OH2	TIP	105	.460	3.133	35.461	1.00	18.93	S
ATOM	2814	OH2	TIP	106	4.603	10.769	51.019	1.00	26.14	S
ATOM	2815	OH2	TIP	107	10.186	8.894	17.137	1.00	16.30	S
ATOM	2816	OH2	TIP	108	-5.744	32.872	22.470	1.00	19.88	S
ATOM	2817	OH2	TIP	109	1.171	43.244	13.267	1.00	20.55	S
ATOM	2818	OH2	TIP	110	13.495	-6.546	28.782	1.00	22.06	S
ATOM	2819	OH2	TIP	111	-7.739	14.581	23.314	1.00	21.61	S
ATOM	2820	OH2	TIP	112	11.516	7.772	5.260	1.00	24.68	S
ATOM	2821	OH2	TIP	113	6.120	-11.567	23.334	1.00	21.24	S
ATOM	2822	OH2	TIP	114	7.436	-8.295	34.334	1.00	18.83	S
ATOM	2823	OH2	TIP	115	-7.736	-6.746	18.652	1.00	20.70	S
ATOM	2824	OH2	TIP	116	-5.415	25.500	34.748	1.00	18.61	S
ATOM	2825	OH2	TIP	117	-2.258	14.277	44.353	1.00	22.24	S
ATOM	2826	OH2	TIP	119	21.949	1.307	37.489	1.00	22.52	S
ATOM	2827	OH2	TIP	120	7.128	8.941	-4.528	1.00	21.21	S
ATOM	2828	OH2	TIP	121	14.744	.270	27.163	1.00	22.34	S
ATOM	2829	OH2	TIP	122	-12.390	3.177	-.844	1.00	24.86	S
ATOM	2830	OH2	TIP	123	9.525	2.327	-.516	1.00	24.48	S
ATOM	2831	OH2	TIP	124	-6.819	13.275	38.743	1.00	20.40	S
ATOM	2832	OH2	TIP	125	-12.817	-1.238	4.959	1.00	22.93	S

ATOM	2833	OH2	TIP	126	2.622	3.976	-6.347	1.00 22.22	S
ATOM	2834	OH2	TIP	127	3.645	-8.212	26.934	1.00 21.83	S
ATOM	2835	OH2	TIP	128	-11.982	.433	3.656	1.00 21.07	S
ATOM	2836	OH2	TIP	129	.586	22.210	46.740	1.00 25.36	S
ATOM	2837	OH2	TIP	130	17.224	3.313	32.344	1.00 13.77	S
ATOM	2838	OH2	TIP	131	23.345	4.436	52.619	1.00 20.13	S
ATOM	2839	OH2	TIP	132	.330	-13.895	26.007	1.00 18.90	S
ATOM	2840	OH2	TIP	133	9.754	-6.683	34.630	1.00 22.45	S
ATOM	2841	OH2	TIP	134	-3.774	-8.055	32.920	1.00 20.45	S
ATOM	2842	OH2	TIP	136	-13.407	-9.343	7.035	1.00 31.83	S
ATOM	2843	OH2	TIP	137	20.758	13.359	33.272	1.00 21.52	S
ATOM	2844	OH2	TIP	138	-1.513	6.528	-8.897	1.00 21.72	S
ATOM	2845	OH2	TIP	139	12.567	32.631	40.633	1.00 26.17	S
ATOM	2846	OH2	TIP	140	-8.570	-10.912	22.657	1.00 16.67	S
ATOM	2847	OH2	TIP	141	17.742	1.030	41.154	1.00 24.30	S
ATOM	2848	OH2	TIP	142	-9.954	7.039	43.979	1.00 21.16	S
ATOM	2849	OH2	TIP	143	-11.980	.409	.609	1.00 25.23	S
ATOM	2850	OH2	TIP	144	17.717	6.606	25.285	1.00 23.04	S
ATOM	2851	OH2	TIP	145	3.129	22.503	20.491	1.00 23.99	S
ATOM	2852	OH2	TIP	146	18.398	6.849	31.971	1.00 22.92	S
ATOM	2853	OH2	TIP	147	-4.874	16.119	37.490	1.00 27.10	S
ATOM	2854	OH2	TIP	148	5.976	-2.037	5.817	1.00 27.95	S
ATOM	2855	OH2	TIP	149	4.233	-9.893	24.749	1.00 17.92	S
ATOM	2856	OH2	TIP	150	-6.650	30.440	19.986	1.00 22.53	S
ATOM	2857	OH2	TIP	152	16.887	24.409	35.093	1.00 29.39	S
ATOM	2858	OH2	TIP	153	-11.070	-.430	38.408	1.00 24.69	S
ATOM	2859	OH2	TIP	154	-20.981	12.570	14.343	1.00 22.94	S
ATOM	2860	OH2	TIP	155	-18.188	1.400	18.283	1.00 21.90	S
ATOM	2861	OH2	TIP	156	-1.888	8.352	48.707	1.00 20.91	S
ATOM	2862	OH2	TIP	157	-6.401	29.700	32.016	1.00 27.73	S
ATOM	2863	OH2	TIP	158	12.523	13.059	27.164	1.00 23.16	S
ATOM	2864	OH2	TIP	159	-18.998	1.532	13.488	1.00 27.51	S
ATOM	2865	OH2	TIP	160	-10.335	6.617	-2.816	1.00 22.50	S
ATOM	2866	OH2	TIP	161	-18.205	-1.939	15.877	1.00 26.60	S
ATOM	2867	OH2	TIP	162	6.873	18.083	-6.633	1.00 23.12	S
ATOM	2868	OH2	TIP	163	11.108	-3.435	21.123	1.00 24.87	S
ATOM	2869	OH2	TIP	164	-6.950	17.939	44.497	1.00 30.07	S
ATOM	2870	OH2	TIP	165	-15.402	-5.839	20.484	1.00 26.16	S
ATOM	2871	OH2	TIP	166	-9.316	30.150	19.391	1.00 20.80	S
ATOM	2872	OH2	TIP	167	-21.084	18.892	22.880	1.00 27.83	S
ATOM	2873	OH2	TIP	168	3.768	14.947	49.832	1.00 17.94	S
ATOM	2874	OH2	TIP	169	2.267	20.740	38.551	1.00 23.09	S
ATOM	2875	OH2	TIP	170	-18.215	8.236	28.965	1.00 26.32	S
ATOM	2876	OH2	TIP	171	-9.931	26.155	-3.699	1.00 28.65	S
ATOM	2877	OH2	TIP	172	-14.952	14.651	32.863	1.00 22.95	S
ATOM	2878	OH2	TIP	173	-2.490	36.021	5.451	1.00 30.83	S
ATOM	2879	OH2	TIP	174	-9.837	-4.584	30.428	1.00 24.27	S
ATOM	2880	OH2	TIP	175	-18.383	23.311	22.650	1.00 24.44	S
ATOM	2881	OH2	TIP	176	3.803	32.144	3.967	1.00 26.80	S
ATOM	2882	OH2	TIP	177	-18.261	17.769	7.285	1.00 19.87	S
ATOM	2883	OH2	TIP	178	-6.038	29.780	36.282	1.00 25.98	S
ATOM	2884	OH2	TIP	179	-7.552	8.686	-5.483	1.00 18.73	S
ATOM	2885	OH2	TIP	180	19.430	2.815	39.284	1.00 20.80	S
ATOM	2886	OH2	TIP	181	23.326	1.757	48.700	1.00 19.79	S
ATOM	2887	OH2	TIP	182	-2.203	19.098	6.712	1.00 22.52	S
ATOM	2888	OH2	TIP	183	15.449	17.346	45.314	1.00 27.39	S
ATOM	2889	OH2	TIP	184	-4.881	15.743	-4.305	1.00 25.54	S
ATOM	2890	OH2	TIP	185	7.086	-.783	12.881	1.00 23.42	S
ATOM	2891	OH2	TIP	186	-7.363	14.083	34.761	1.00 19.39	S
ATOM	2892	OH2	TIP	187	16.111	4.209	19.980	1.00 26.52	S

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ATOM   2893  OH2 TIP   188     -15.185  17.358  32.184  1.00 28.44      S
ATOM   2894  OH2 TIP   189     -21.385  20.176  17.585  1.00 18.75      S
ATOM   2895  OH2 TIP   190      14.844  -1.244  29.817  1.00 21.50      S
ATOM   2896  OH2 TIP   191      10.591  26.020  43.366  1.00 28.91      S
ATOM   2897  OH2 TIP   192      -7.713  36.463  10.318  1.00 25.82      S
ATOM   2898  OH2 TIP   193      11.482  -1.349  42.668  1.00 23.23      S
ATOM   2899  OH2 TIP   194       6.407  -8.890  18.408  1.00 19.79      S
ATOM   2900  OH2 TIP   195       8.900   3.561   1.780  1.00 23.64      S
ATOM   2901  OH2 TIP   196      -9.728  -9.430  32.396  1.00 30.35      S
ATOM   2902  OH2 TIP   197      23.746  13.274  34.443  1.00 22.07      S
ATOM   2903  OH2 TIP   198       9.995  28.759  41.514  1.00 26.09      S
ATOM   2904  OH2 TIP   199       5.009  19.549  21.181  1.00 30.58      S
ATOM   2905  OH2 TIP   200      25.038  15.296  42.041  1.00 29.50      S
ATOM   2906  OH2 TIP   201     -10.048  -8.409  28.603  1.00 28.07      S
ATOM   2907  OH2 TIP   202     -17.617    .690  15.796  1.00 22.01      S
ATOM   2908  OH2 TIP   203       1.005   6.413 -10.219  1.00 22.96      S
ATOM   2909  OH2 TIP   204       1.164  -9.392  30.631  1.00 23.26      S
ATOM   2910  OH2 TIP   205     -21.323   5.667  14.158  1.00 25.83      S
ATOM   2911  OH2 TIP   206      11.821  18.221  17.545  1.00 29.64      S
ATOM   2912  OH2 TIP   207       7.793  14.504  -4.041  1.00 25.65      S
ATOM   2913  OH2 TIP   208      -3.103  27.649  20.677  1.00 18.80      S
ATOM   2914  OH2 TIP   209     -21.678   8.150  16.308  1.00 24.85      S
ATOM   2915  OH2 TIP   210      18.006  12.362  49.464  1.00 26.62      S
ATOM   2916  OH2 TIP   211     -16.155  -5.271  17.688  1.00 23.43      S
ATOM   2917  OH2 TIP   212       3.682  29.153   7.462  1.00 25.58      S
ATOM   2918  OH2 TIP   213     -12.248  25.037  31.720  1.00 28.21      S
ATOM   2919  OH2 TIP   214     -14.222  29.793  20.553  1.00 30.08      S
ATOM   2920  OH2 TIP   215      20.787  20.184  34.443  1.00 28.87      S
ATOM   2921  OH2 TIP   216      -2.086  31.821  37.384  1.00 28.40      S
ATOM   2922  OH2 TIP   217      24.474   2.473  45.521  1.00 26.98      S
ATOM   2923  OH2 TIP   218       5.066  16.366  11.838  1.00 27.12      S
ATOM   2924  OH2 TIP   219      -2.789  20.555  53.528  1.00 30.92      S
ATOM   2925  OH2 TIP   220       7.858   1.904   3.261  1.00 28.74      S
ATOM   2926  OH2 TIP   221     -13.132  14.703  35.191  1.00 26.36      S
ATOM   2927  OH2 TIP   222      12.424   1.824  46.175  1.00 23.73      S
ATOM   2928  OH2 TIP   223      -9.749  22.573  34.313  1.00 24.03      S
ATOM   2929  OH2 TIP   224      -1.931  -7.163  13.015  1.00 22.40      S
ATOM   2930  OH2 TIP   225       2.619  22.080  41.877  1.00 27.86      S
ATOM   2931  OH2 TIP   226      -6.472  28.316  33.973  1.00 24.68      S
ATOM   2932  OH2 TIP   227     -11.822  -7.268   6.157  1.00 26.46      S
ATOM   2933  OH2 TIP   228      13.888   9.027   9.906  1.00 24.14      S
ATOM   2934  OH2 TIP   229       -.089   1.763  40.836  1.00 27.96      S
ATOM   2935  OH2 TIP   230      14.960  26.472  36.959  1.00 21.01      S
ATOM   2936  OH2 TIP   231      12.205  19.536  46.718  1.00 26.19      S
ATOM   2937  OH2 TIP   232       9.952  -3.873  36.178  1.00 28.34      S
ATOM   2938  OH2 TIP   233      12.502   3.057  17.466  1.00 23.30      S
ATOM   2939  OH2 TIP   234      -6.023   4.372  -8.018  1.00 31.92      S
ATOM   2940  OH2 TIP   235       1.098  17.563  18.913  1.00 25.00      S
ATOM   2941  OH2 TIP   236       6.052  24.879  25.870  1.00 26.69      S
END
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Table 3

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REMARK GnT I "be"  Structure of rabbit GnT I bound to UDP-GlcNAc and a
REMARK Manganese 2+ ion.  Ulug Unligil & Dr. James Rini, Oct 25, 1999
REMARK coordinates from minimization refinement
REMARK refinement resolution: 50.0 - 1.8 A
REMARK starting r= 0.2006 free_r= 0.2388
REMARK final     r= 0.1987 free_r= 0.2388
REMARK rmsd bonds= 0.006698  rmsd angles=  1.36297
REMARK wa= 1.4
REMARK target= mlf cycles= 1 steps= 200
REMARK sg= P2(1)2(1)2(1) a= 40.541 b= 82.190 c= 101.956 alpha= 90 beta= 90 gamma=
90
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:ion.param
REMARK parameter file 3  : ../../data/udpglcnac.param
REMARK parameter file 4  : ../../data/glycerol.param
REMARK parameter file 5  : CNS_TOPPAR:water_rep.param
REMARK molecular structure file: ../alternate.mtf
REMARK input coordinates: bindividual.bi4.10.pdb
REMARK reflection file= ../../data/gntlbe.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.8
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   4.245 B22=   1.052 B33=  -5.296
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:   -1.075
REMARK bulk solvent: density level= 0.415966 e/A^3, B-factor= 55.91 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range:     61022 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  18103 (  29.7 % )
REMARK number of reflections rejected:                            0 (   0.0 % )
REMARK total number of reflections used:                      42919 (  70.3 % )
REMARK number of reflections in working set:                  40743 (  66.8 % )
REMARK number of reflections in test set:                      2176 (   3.6 % )
CRYST1   40.541   82.190  101.956  90.00  90.00  90.00 P 21 21 21
REMARK FILENAME="minimize.bi4.14.pdb"
REMARK DATE:22-Oct-1999  02:45:19       created by user: ulu
REMARK VERSION:0.9a
ATOM      1  CB  ALA   106      -17.101  -1.137  17.571  1.00 30.47
ATOM      2  C   ALA   106      -16.456  -1.044  15.162  1.00 28.96
ATOM      3  O   ALA   106      -15.343  -1.514  15.382  1.00 29.71
ATOM      4  N   ALA   106      -18.199  -2.631  15.920  1.00 30.66
ATOM      5  CA  ALA   106      -17.604  -1.274  16.134  1.00 30.14
ATOM      6  N   VAL   107      -16.730  -0.319  14.084  1.00 28.66
ATOM      7  CA  VAL   107      -15.710  -0.038  13.085  1.00 26.78
ATOM      8  CB  VAL   107      -16.351   0.168  11.698  1.00 27.43
ATOM      9  CG1 VAL   107      -15.284   0.499  10.672  1.00 26.59
ATOM     10  CG2 VAL   107      -17.108  -1.089  11.290  1.00 27.37
ATOM     11  C   VAL   107      -14.924   1.211  13.475  1.00 26.03
ATOM     12  O   VAL   107      -15.505   2.282  13.664  1.00 27.13
ATOM     13  N   ILE   108      -13.606   1.065  13.591  1.00 22.67
ATOM     14  CA  ILE   108      -12.728   2.176  13.965  1.00 18.77
ATOM     15  CB  ILE   108      -11.839   1.807  15.171  1.00 17.32
ATOM     16  CG2 ILE   108      -10.946   2.994  15.548  1.00 18.32
ATOM     17  CG1 ILE   108      -12.716   1.418  16.363  1.00 17.51
ATOM     18  CD1 ILE   108      -11.924   0.929  17.571  1.00 15.69
ATOM     19  C   ILE   108      -11.823   2.540  12.794  1.00 15.99
ATOM     20  O   ILE   108      -10.849   1.843  12.508  1.00 16.54
ATOM     21  N   PRO   109      -12.134   3.644  12.101  1.00 15.66
ATOM     22  CD  PRO   109      -13.308   4.522  12.282  1.00 14.05
ATOM     23  CA  PRO   109      -11.334   4.080  10.956  1.00 13.53
ATOM     24  CB  PRO   109      -12.276   5.030  10.232  1.00 14.35
ATOM     25  CG  PRO   109      -12.982   5.693  11.378  1.00 14.63
ATOM     26  C   PRO   109      -10.035   4.767  11.347  1.00 12.80
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ATOM	27	O	PRO	109	-9.930	5.396	12.412	1.00	10.08	
ATOM	28	N	ILE	110	-9.033	4.609	10.493	1.00	11.34	
ATOM	29	CA	ILE	110	-7.760	5.261	10.713	1.00	10.09	
ATOM	30	CB	ILE	110	-6.559	4.370	10.328	1.00	10.10	
ATOM	31	CG2	ILE	110	-5.244	5.087	10.678	1.00	5.90	
ATOM	32	CG1	ILE	110	-6.653	3.019	11.036	1.00	6.06	
ATOM	33	CD1	ILE	110	-6.681	3.093	12.559	1.00	9.66	
ATOM	34	C	ILE	110	-7.821	6.422	9.738	1.00	10.73	
ATOM	35	O	ILE	110	-7.929	6.212	8.524	1.00	10.77	
ATOM	36	N	LEU	111	-7.789	7.640	10.267	1.00	8.99	
ATOM	37	CA	LEU	111	-7.822	8.827	9.429	1.00	8.61	
ATOM	38	CB	LEU	111	-8.666	9.931	10.074	1.00	9.18	
ATOM	39	CG	LEU	111	-8.544	11.325	9.445	1.00	11.48	
ATOM	40	CD1	LEU	111	-8.923	11.271	7.971	1.00	7.83	
ATOM	41	CD2	LEU	111	-9.438	12.298	10.189	1.00	7.99	
ATOM	42	C	LEU	111	-6.388	9.303	9.273	1.00	10.07	
ATOM	43	O	LEU	111	-5.775	9.773	10.229	1.00	6.50	
ATOM	44	N	VAL	112	-5.851	9.145	8.069	1.00	7.32	
ATOM	45	CA	VAL	112	-4.493	9.578	7.771	1.00	8.69	
ATOM	46	CB	VAL	112	-3.807	8.617	6.763	1.00	11.40	
ATOM	47	CG1	VAL	112	-2.432	9.136	6.383	1.00	10.29	
ATOM	48	CG2	VAL	112	-3.686	7.223	7.369	1.00	5.18	
ATOM	49	C	VAL	112	-4.522	10.992	7.182	1.00	8.90	
ATOM	50	O	VAL	112	-5.192	11.246	6.173	1.00	9.08	
ATOM	51	N	ILE	113	-3.796	11.905	7.818	0.50	8.75	AC1
ATOM	52	CA	ILE	113	-3.723	13.290	7.368	0.50	8.89	AC1
ATOM	53	CB	ILE	113	-3.676	14.276	8.565	0.50	9.80	AC1
ATOM	54	CG2	ILE	113	-3.469	15.704	8.065	0.50	9.83	AC1
ATOM	55	CG1	ILE	113	-4.982	14.197	9.365	0.50	9.27	AC1
ATOM	56	CD1	ILE	113	-5.236	12.854	10.010	0.50	11.40	AC1
ATOM	57	C	ILE	113	-2.464	13.445	6.525	0.50	9.09	AC1
ATOM	58	O	ILE	113	-1.359	13.150	6.984	0.50	8.54	AC1
ATOM	59	N	ALA	114	-2.643	13.901	5.288	1.00	9.09	
ATOM	60	CA	ALA	114	-1.532	14.078	4.355	1.00	10.74	
ATOM	61	CB	ALA	114	-1.553	12.937	3.312	1.00	9.90	
ATOM	62	C	ALA	114	-1.595	15.428	3.647	1.00	10.78	
ATOM	63	O	ALA	114	-2.603	16.129	3.728	1.00	9.19	
ATOM	64	N	CYS	115	-0.521	15.781	2.937	1.00	12.39	
ATOM	65	CA	CYS	115	-0.460	17.059	2.221	1.00	13.37	
ATOM	66	C	CYS	115	0.476	17.047	1.015	1.00	14.11	
ATOM	67	O	CYS	115	0.032	16.870	-0.128	1.00	13.25	
ATOM	68	CB	CYS	115	-0.044	18.167	3.199	1.00	14.31	
ATOM	69	SG	CYS	115	0.483	19.792	2.547	1.00	12.75	
ATOM	70	N	ASP	116	1.772	17.219	1.266	1.00	13.60	
ATOM	71	CA	ASP	116	2.740	17.264	0.180	1.00	13.58	
ATOM	72	CB	ASP	116	3.129	18.725	-0.101	1.00	13.69	
ATOM	73	CG	ASP	116	3.725	19.428	1.115	1.00	14.92	
ATOM	74	OD1	ASP	116	3.846	20.670	1.077	1.00	14.80	
ATOM	75	OD2	ASP	116	4.083	18.753	2.102	1.00	12.59	
ATOM	76	C	ASP	116	4.001	16.438	0.372	1.00	13.59	
ATOM	77	O	ASP	116	5.042	16.754	-0.218	1.00	13.40	
ATOM	78	N	ARG	117	3.924	15.395	1.195	1.00	10.72	
ATOM	79	CA	ARG	117	5.077	14.531	1.418	1.00	11.10	
ATOM	80	CB	ARG	117	5.419	14.455	2.915	1.00	9.78	
ATOM	81	CG	ARG	117	6.088	15.723	3.451	1.00	11.64	
ATOM	82	CD	ARG	117	6.509	15.600	4.924	1.00	11.53	
ATOM	83	NE	ARG	117	5.374	15.378	5.812	1.00	13.33	
ATOM	84	CZ	ARG	117	5.314	15.805	7.070	1.00	11.66	
ATOM	85	NH1	ARG	117	6.334	16.491	7.591	1.00	10.56	
ATOM	86	NH2	ARG	117	4.241	15.542	7.808	1.00	8.60	
ATOM	87	C	ARG	117	4.782	13.140	0.869	1.00	11.54	
ATOM	88	O	ARG	117	3.857	12.458	1.329	1.00	11.01	
ATOM	89	N	SER	118	5.572	12.726	-0.117	1.00	11.85	
ATOM	90	CA	SER	118	5.405	11.421	-0.742	1.00	12.53	
ATOM	91	CB	SER	118	6.305	11.292	-1.976	1.00	11.85	
ATOM	92	OG	SER	118	7.671	11.447	-1.628	1.00	15.63	
ATOM	93	C	SER	118	5.707	10.296	0.226	1.00	12.63	

ATOM	94	O	SER	118	5.302	9.155	-0.006	1.00	13.89
ATOM	95	N	THR	119	6.412	10.616	1.308	1.00	12.37
ATOM	96	CA	THR	119	6.752	9.622	2.315	1.00	11.71
ATOM	97	CB	THR	119	7.803	10.161	3.307	1.00	12.47
ATOM	98	OG1	THR	119	7.360	11.408	3.850	1.00	12.53
ATOM	99	CG2	THR	119	9.142	10.370	2.603	1.00	9.00
ATOM	100	C	THR	119	5.514	9.146	3.083	1.00	13.85
ATOM	101	O	THR	119	5.616	8.396	4.065	1.00	11.67
ATOM	102	N	VAL	120	4.341	9.599	2.651	1.00	12.01
ATOM	103	CA	VAL	120	3.111	9.137	3.267	1.00	12.00
ATOM	104	CB	VAL	120	1.867	9.851	2.666	1.00	11.81
ATOM	105	CG1	VAL	120	1.795	9.610	1.158	1.00	10.65
ATOM	106	CG2	VAL	120	0.596	9.348	3.350	1.00	11.58
ATOM	107	C	VAL	120	3.097	7.636	2.925	1.00	11.66
ATOM	108	O	VAL	120	2.378	6.844	3.534	1.00	9.69
ATOM	109	N	ARG	121	3.922	7.263	1.943	1.00	10.91
ATOM	110	CA	ARG	121	4.061	5.871	1.515	1.00	11.87
ATOM	111	CB	ARG	121	5.099	5.765	0.383	1.00	11.58
ATOM	112	CG	ARG	121	5.359	4.340	-0.121	1.00	14.15
ATOM	113	CD	ARG	121	6.484	4.303	-1.169	1.00	14.21
ATOM	114	NE	ARG	121	6.131	4.982	-2.414	1.00	16.64
ATOM	115	CZ	ARG	121	5.334	4.477	-3.351	1.00	16.42
ATOM	116	NH1	ARG	121	4.796	3.273	-3.192	1.00	16.90
ATOM	117	NH2	ARG	121	5.080	5.175	-4.454	1.00	15.44
ATOM	118	C	ARG	121	4.507	5.012	2.700	1.00	12.00
ATOM	119	O	ARG	121	3.938	3.956	2.967	1.00	10.47
ATOM	120	N	ARG	122	5.526	5.472	3.418	1.00	12.89
ATOM	121	CA	ARG	122	6.029	4.736	4.567	1.00	11.41
ATOM	122	CB	ARG	122	7.239	5.460	5.163	1.00	14.50
ATOM	123	CG	ARG	122	7.820	4.823	6.411	1.00	12.95
ATOM	124	CD	ARG	122	9.071	5.573	6.860	1.00	16.67
ATOM	125	NE	ARG	122	9.519	5.133	8.180	1.00	17.60
ATOM	126	CZ	ARG	122	10.636	5.547	8.772	1.00	20.29
ATOM	127	NH1	ARG	122	11.435	6.413	8.161	1.00	20.12
ATOM	128	NH2	ARG	122	10.948	5.110	9.986	1.00	17.47
ATOM	129	C	ARG	122	4.940	4.568	5.613	1.00	11.78
ATOM	130	O	ARG	122	4.816	3.503	6.224	1.00	8.82
ATOM	131	N	CYS	123	4.149	5.619	5.819	1.00	11.42
ATOM	132	CA	CYS	123	3.059	5.575	6.784	1.00	10.90
ATOM	133	CB	CYS	123	2.385	6.952	6.885	1.00	11.59
ATOM	134	SG	CYS	123	0.899	7.021	7.936	1.00	9.51
ATOM	135	C	CYS	123	2.037	4.526	6.364	1.00	11.98
ATOM	136	O	CYS	123	1.685	3.643	7.150	1.00	11.01
ATOM	137	N	LEU	124	1.583	4.606	5.114	1.00	11.43
ATOM	138	CA	LEU	124	0.584	3.672	4.618	1.00	10.28
ATOM	139	CB	LEU	124	0.056	4.118	3.241	1.00	10.68
ATOM	140	CG	LEU	124	-0.798	5.402	3.181	1.00	9.75
ATOM	141	CD1	LEU	124	-1.271	5.641	1.751	1.00	11.34
ATOM	142	CD2	LEU	124	-2.005	5.268	4.101	1.00	8.96
ATOM	143	C	LEU	124	1.086	2.232	4.551	1.00	10.40
ATOM	144	O	LEU	124	0.345	1.312	4.890	1.00	10.23
ATOM	145	N	ASP	125	2.333	2.025	4.129	1.00	10.09
ATOM	146	CA	ASP	125	2.852	0.663	4.051	1.00	12.17
ATOM	147	CB	ASP	125	4.320	0.639	3.600	1.00	12.37
ATOM	148	CG	ASP	125	4.493	0.979	2.123	1.00	12.18
ATOM	149	OD1	ASP	125	3.523	0.860	1.338	1.00	10.25
ATOM	150	OD2	ASP	125	5.620	1.353	1.741	1.00	10.36
ATOM	151	C	ASP	125	2.725	-0.060	5.390	1.00	12.61
ATOM	152	O	ASP	125	2.190	-1.166	5.447	1.00	11.20
ATOM	153	N	LYS	126	3.188	0.578	6.464	1.00	13.37
ATOM	154	CA	LYS	126	3.136	-0.023	7.798	1.00	14.20
ATOM	155	CB	LYS	126	3.926	0.830	8.789	1.00	16.31
ATOM	156	CG	LYS	126	5.436	0.771	8.599	1.00	17.93
ATOM	157	CD	LYS	126	5.949	-0.653	8.789	1.00	18.55
ATOM	158	CE	LYS	126	7.466	-0.721	8.692	1.00	20.62
ATOM	159	NZ	LYS	126	7.982	-0.271	7.366	1.00	19.78
ATOM	160	C	LYS	126	1.725	-0.252	8.335	1.00	13.42

ATOM	161	O	LYS	126	1.451	-1.290	8.938	1.00	14.49
ATOM	162	N	LEU	127	0.832	0.712	8.124	1.00	12.44
ATOM	163	CA	LEU	127	-0.548	0.585	8.588	1.00	13.07
ATOM	164	CB	LEU	127	-1.349	1.849	8.259	1.00	12.39
ATOM	165	CG	LEU	127	-1.239	3.072	9.163	1.00	12.08
ATOM	166	CD1	LEU	127	-1.874	4.277	8.469	1.00	11.74
ATOM	167	CD2	LEU	127	-1.938	2.794	10.480	1.00	7.81
ATOM	168	C	LEU	127	-1.223	-0.597	7.910	1.00	13.53
ATOM	169	O	LEU	127	-1.876	-1.412	8.555	1.00	14.28
ATOM	170	N	LEU	128	-1.071	-0.665	6.592	1.00	13.43
ATOM	171	CA	LEU	128	-1.668	-1.725	5.801	1.00	13.03
ATOM	172	CB	LEU	128	-1.541	-1.390	4.310	1.00	12.98
ATOM	173	CG	LEU	128	-2.518	-0.327	3.811	1.00	13.48
ATOM	174	CD1	LEU	128	-2.154	0.110	2.386	1.00	10.66
ATOM	175	CD2	LEU	128	-3.930	-0.909	3.850	1.00	13.10
ATOM	176	C	LEU	128	-1.021	-3.065	6.094	1.00	13.08
ATOM	177	O	LEU	128	-1.673	-4.106	6.031	1.00	13.70
ATOM	178	N	HIS	129	0.266	-3.040	6.420	1.00	14.33
ATOM	179	CA	HIS	129	0.971	-4.277	6.714	1.00	14.32
ATOM	180	CB	HIS	129	2.472	-4.020	6.830	1.00	16.63
ATOM	181	CG	HIS	129	3.268	-5.252	7.136	1.00	19.33
ATOM	182	CD2	HIS	129	3.739	-5.739	8.308	1.00	20.57
ATOM	183	ND1	HIS	129	3.616	-6.173	6.171	1.00	21.42
ATOM	184	CE1	HIS	129	4.267	-7.174	6.736	1.00	20.41
ATOM	185	NE2	HIS	129	4.355	-6.936	8.032	1.00	21.50
ATOM	186	C	HIS	129	0.469	-4.903	8.009	1.00	14.82
ATOM	187	O	HIS	129	0.271	-6.113	8.090	1.00	13.73
ATOM	188	N	TYR	130	0.253	-4.068	9.018	1.00	13.47
ATOM	189	CA	TYR	130	-0.192	-4.541	10.321	1.00	15.97
ATOM	190	CB	TYR	130	0.401	-3.643	11.410	1.00	15.46
ATOM	191	CG	TYR	130	1.901	-3.786	11.551	1.00	17.64
ATOM	192	CD1	TYR	130	2.726	-2.663	11.643	1.00	17.40
ATOM	193	CE1	TYR	130	4.109	-2.794	11.767	1.00	17.72
ATOM	194	CD2	TYR	130	2.497	-5.048	11.589	1.00	16.37
ATOM	195	CE2	TYR	130	3.876	-5.190	11.715	1.00	18.08
ATOM	196	CZ	TYR	130	4.676	-4.060	11.804	1.00	18.48
ATOM	197	OH	TYR	130	6.042	-4.202	11.949	1.00	20.65
ATOM	198	C	TYR	130	-1.701	-4.647	10.518	1.00	15.03
ATOM	199	O	TYR	130	-2.155	-5.340	11.421	1.00	17.48
ATOM	200	N	ARG	131	-2.479	-3.964	9.688	1.00	14.80
ATOM	201	CA	ARG	131	-3.934	-3.997	9.830	1.00	13.16
ATOM	202	CB	ARG	131	-4.595	-3.271	8.654	1.00	11.16
ATOM	203	CG	ARG	131	-6.101	-3.224	8.766	1.00	12.50
ATOM	204	CD	ARG	131	-6.725	-2.190	7.843	1.00	10.33
ATOM	205	NE	ARG	131	-6.575	-2.533	6.436	1.00	10.56
ATOM	206	CZ	ARG	131	-7.249	-1.937	5.460	1.00	11.25
ATOM	207	NH1	ARG	131	-8.115	-0.976	5.754	1.00	12.04
ATOM	208	NH2	ARG	131	-7.065	-2.300	4.197	1.00	10.98
ATOM	209	C	ARG	131	-4.457	-5.434	9.920	1.00	13.13
ATOM	210	O	ARG	131	-4.253	-6.234	9.007	1.00	12.63
ATOM	211	N	PRO	132	-5.131	-5.785	11.032	1.00	13.39
ATOM	212	CD	PRO	132	-5.158	-5.073	12.323	1.00	12.76
ATOM	213	CA	PRO	132	-5.658	-7.147	11.185	1.00	12.07
ATOM	214	CB	PRO	132	-5.768	-7.297	12.700	1.00	12.23
ATOM	215	CG	PRO	132	-6.128	-5.906	13.135	1.00	13.77
ATOM	216	C	PRO	132	-6.992	-7.401	10.489	1.00	13.90
ATOM	217	O	PRO	132	-7.402	-8.548	10.310	1.00	11.86
ATOM	218	N	SER	133	-7.669	-6.325	10.103	1.00	14.50
ATOM	219	CA	SER	133	-8.963	-6.436	9.451	1.00	15.64
ATOM	220	CB	SER	133	-10.046	-6.723	10.491	1.00	15.57
ATOM	221	OG	SER	133	-11.341	-6.507	9.955	1.00	15.66
ATOM	222	C	SER	133	-9.311	-5.158	8.723	1.00	16.59
ATOM	223	O	SER	133	-9.398	-4.098	9.341	1.00	14.39
ATOM	224	N	ALA	134	-9.529	-5.271	7.414	1.00	16.76
ATOM	225	CA	ALA	134	-9.886	-4.125	6.591	1.00	16.91
ATOM	226	CB	ALA	134	-9.888	-4.525	5.120	1.00	17.70
ATOM	227	C	ALA	134	-11.255	-3.579	6.981	1.00	17.67

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ATOM    228  O   ALA   134     -11.464   -2.366    7.001  1.00 17.12
ATOM    229  N   GLU   135     -12.190   -4.477    7.290  1.00 17.82
ATOM    230  CA  GLU   135     -13.537   -4.063    7.671  1.00 20.07
ATOM    231  CB  GLU   135     -14.496   -5.265    7.700  1.00 23.40
ATOM    232  CG  GLU   135     -13.824   -6.632    7.802  1.00 29.26
ATOM    233  CD  GLU   135     -13.223   -7.088    6.483  1.00 31.22
ATOM    234  OE1 GLU   135     -13.983   -7.196    5.497  1.00 32.45
ATOM    235  OE2 GLU   135     -11.996   -7.338    6.428  1.00 31.71
ATOM    236  C   GLU   135     -13.581   -3.347    9.015  1.00 17.82
ATOM    237  O   GLU   135     -14.340   -2.398    9.190  1.00 17.22
ATOM    238  N   LEU   136     -12.769   -3.795    9.965  1.00 17.63
ATOM    239  CA  LEU   136     -12.747   -3.169   11.281  1.00 17.38
ATOM    240  CB  LEU   136     -12.149   -4.124   12.313  1.00 19.32
ATOM    241  CG  LEU   136     -12.968   -5.399   12.542  1.00 21.75
ATOM    242  CD1 LEU   136     -12.324   -6.226   13.644  1.00 20.10
ATOM    243  CD2 LEU   136     -14.404   -5.029   12.918  1.00 21.27
ATOM    244  C   LEU   136     -11.972   -1.860   11.291  1.00 17.01
ATOM    245  O   LEU   136     -12.320   -0.932   12.028  1.00 14.10
ATOM    246  N   PHE   137     -10.926   -1.788   10.469  1.00 15.95
ATOM    247  CA  PHE   137     -10.100   -0.592   10.387  1.00 14.04
ATOM    248  CB  PHE   137      -8.696   -0.872   10.933  1.00 14.43
ATOM    249  CG  PHE   137      -8.677   -1.251   12.381  1.00 17.23
ATOM    250  CD1 PHE   137      -8.736   -2.584   12.764  1.00 17.24
ATOM    251  CD2 PHE   137      -8.623   -0.268   13.368  1.00 17.96
ATOM    252  CE1 PHE   137      -8.741   -2.939   14.111  1.00 17.93
ATOM    253  CE2 PHE   137      -8.627   -0.616   14.720  1.00 17.87
ATOM    254  CZ  PHE   137      -8.687   -1.953   15.088  1.00 15.35
ATOM    255  C   PHE   137      -9.966   -0.009    8.984  1.00 12.32
ATOM    256  O   PHE   137      -8.899   -0.086    8.375  1.00 11.51
ATOM    257  N   PRO   138     -11.040    0.594    8.454  1.00 11.30
ATOM    258  CD  PRO   138     -12.384    0.807    9.017  1.00 11.44
ATOM    259  CA  PRO   138     -10.938    1.172    7.112  1.00 10.64
ATOM    260  CB  PRO   138     -12.373    1.590    6.802  1.00  9.00
ATOM    261  CG  PRO   138     -12.917    1.923    8.153  1.00 12.10
ATOM    262  C   PRO   138      -9.993    2.361    7.198  1.00 10.58
ATOM    263  O   PRO   138     -10.024    3.114    8.171  1.00 10.01
ATOM    264  N   ILE   139      -9.150    2.518    6.189  1.00  9.44
ATOM    265  CA  ILE   139      -8.188    3.609    6.164  1.00  8.45
ATOM    266  CB  ILE   139      -6.808    3.098    5.692  1.00  9.09
ATOM    267  CG2 ILE   139      -5.849    4.279    5.447  1.00  8.51
ATOM    268  CG1 ILE   139      -6.246    2.125    6.734  1.00  8.77
ATOM    269  CD1 ILE   139      -5.041    1.358    6.254  1.00 12.13
ATOM    270  C   ILE   139      -8.682    4.707    5.238  1.00  8.57
ATOM    271  O   ILE   139      -8.948    4.476    4.058  1.00  9.55
ATOM    272  N   ILE   140      -8.821    5.903    5.789  1.00  9.27
ATOM    273  CA  ILE   140      -9.276    7.047    5.019  1.00  8.88
ATOM    274  CB  ILE   140     -10.531    7.692    5.670  1.00 10.08
ATOM    275  CG2 ILE   140     -10.796    9.053    5.067  1.00  8.95
ATOM    276  CG1 ILE   140     -11.765    6.802    5.450  1.00 11.30
ATOM    277  CD1 ILE   140     -11.721    5.484    6.170  1.00 13.03
ATOM    278  C   ILE   140      -8.129    8.044    5.005  1.00 10.44
ATOM    279  O   ILE   140      -7.733    8.560    6.052  1.00 13.07
ATOM    280  N   VAL   141      -7.577    8.291    3.821  1.00 11.13
ATOM    281  CA  VAL   141      -6.474    9.232    3.675  1.00  9.57
ATOM    282  CB  VAL   141      -5.463    8.753    2.606  1.00  9.75
ATOM    283  CG1 VAL   141      -4.210    9.640    2.626  1.00  9.74
ATOM    284  CG2 VAL   141      -5.095    7.297    2.852  1.00  7.84
ATOM    285  C   VAL   141      -7.036   10.578    3.238  1.00  9.88
ATOM    286  O   VAL   141      -7.554   10.711    2.127  1.00  8.29
ATOM    287  N   SER   142      -6.961   11.573    4.114  1.00 10.53
ATOM    288  CA  SER   142      -7.455   12.902    3.766  1.00  9.39
ATOM    289  CB  SER   142      -8.145   13.560    4.965  1.00 10.44
ATOM    290  OG  SER   142      -8.849   14.734    4.574  1.00  9.14
ATOM    291  C   SER   142      -6.252   13.721    3.325  1.00 11.28
ATOM    292  O   SER   142      -5.337   13.980    4.111  1.00 11.70
ATOM    293  N   GLN   143      -6.239   14.107    2.056  1.00  8.36
ATOM    294  CA  GLN   143      -5.134   14.890    1.541  1.00 11.82
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ATOM	295	CB	GLN	143	-4.585	14.290	0.243	1.00	11.19
ATOM	296	CG	GLN	143	-3.508	15.180	-0.349	1.00	13.74
ATOM	297	CD	GLN	143	-3.004	14.742	-1.703	1.00	13.54
ATOM	298	OE1	GLN	143	-3.723	14.122	-2.487	1.00	13.25
ATOM	299	NE2	GLN	143	-1.759	15.093	-1.997	1.00	13.46
ATOM	300	C	GLN	143	-5.518	16.340	1.287	1.00	11.48
ATOM	301	O	GLN	143	-6.524	16.630	0.637	1.00	12.67
ATOM	302	N	ASP	144	-4.696	17.241	1.810	1.00	11.58
ATOM	303	CA	ASP	144	-4.867	18.682	1.659	1.00	13.30
ATOM	304	CB	ASP	144	-4.680	19.332	3.044	1.00	12.47
ATOM	305	CG	ASP	144	-4.759	20.850	3.021	1.00	13.17
ATOM	306	OD1	ASP	144	-5.463	21.418	2.168	1.00	10.32
ATOM	307	OD2	ASP	144	-4.125	21.483	3.894	1.00	15.78
ATOM	308	C	ASP	144	-3.746	19.090	0.692	1.00	12.95
ATOM	309	O	ASP	144	-2.998	18.229	0.222	1.00	11.46
ATOM	310	N	CYS	145	-3.660	20.374	0.360	1.00	12.81
ATOM	311	CA	CYS	145	-2.573	20.877	-0.482	1.00	15.10
ATOM	312	C	CYS	145	-2.562	20.599	-1.985	1.00	17.30
ATOM	313	O	CYS	145	-1.945	21.347	-2.734	1.00	18.23
ATOM	314	CB	CYS	145	-1.253	20.404	0.123	1.00	14.98
ATOM	315	SG	CYS	145	-1.216	20.700	1.920	1.00	17.00
ATOM	316	N	GLY	146	-3.208	19.528	-2.428	1.00	16.85
ATOM	317	CA	GLY	146	-3.227	19.229	-3.851	1.00	18.62
ATOM	318	C	GLY	146	-1.884	18.901	-4.494	1.00	18.93
ATOM	319	O	GLY	146	-1.673	19.184	-5.672	1.00	20.07
ATOM	320	N	HIS	147	-0.974	18.301	-3.731	1.00	17.21
ATOM	321	CA	HIS	147	0.348	17.930	-4.240	1.00	16.59
ATOM	322	CB	HIS	147	1.261	17.588	-3.055	1.00	15.25
ATOM	323	CG	HIS	147	2.699	17.375	-3.418	1.00	14.02
ATOM	324	CD2	HIS	147	3.716	18.254	-3.588	1.00	15.16
ATOM	325	ND1	HIS	147	3.247	16.121	-3.593	1.00	12.79
ATOM	326	CE1	HIS	147	4.538	16.237	-3.851	1.00	11.50
ATOM	327	NE2	HIS	147	4.848	17.521	-3.853	1.00	10.92
ATOM	328	C	HIS	147	0.150	16.718	-5.148	1.00	17.31
ATOM	329	O	HIS	147	-0.174	15.632	-4.672	1.00	16.87
ATOM	330	N	GLU	148	0.350	16.911	-6.451	1.00	17.53
ATOM	331	CA	GLU	148	0.153	15.853	-7.447	1.00	18.64
ATOM	332	CB	GLU	148	0.554	16.359	-8.839	1.00	22.11
ATOM	333	CG	GLU	148	0.275	15.375	-9.971	1.00	26.46
ATOM	334	CD	GLU	148	-1.173	14.917	-10.000	1.00	31.18
ATOM	335	OE1	GLU	148	-2.070	15.766	-9.799	1.00	33.78
ATOM	336	OE2	GLU	148	-1.419	13.710	-10.234	1.00	32.81
ATOM	337	C	GLU	148	0.868	14.532	-7.173	1.00	17.38
ATOM	338	O	GLU	148	0.245	13.470	-7.196	1.00	16.26
ATOM	339	N	GLU	149	2.172	14.588	-6.929	1.00	15.43
ATOM	340	CA	GLU	149	2.922	13.368	-6.675	1.00	17.64
ATOM	341	CB	GLU	149	4.405	13.676	-6.488	1.00	20.36
ATOM	342	CG	GLU	149	5.232	12.457	-6.153	1.00	22.80
ATOM	343	CD	GLU	149	6.709	12.772	-6.070	1.00	25.67
ATOM	344	OE1	GLU	149	7.459	11.975	-5.466	1.00	26.81
ATOM	345	OE2	GLU	149	7.117	13.816	-6.620	1.00	29.49
ATOM	346	C	GLU	149	2.396	12.632	-5.453	1.00	16.92
ATOM	347	O	GLU	149	2.254	11.411	-5.469	1.00	16.82
ATOM	348	N	THR	150	2.107	13.372	-4.390	1.00	16.57
ATOM	349	CA	THR	150	1.591	12.742	-3.188	1.00	14.84
ATOM	350	CB	THR	150	1.462	13.750	-2.039	1.00	13.99
ATOM	351	OG1	THR	150	2.763	14.272	-1.707	1.00	11.67
ATOM	352	CG2	THR	150	0.874	13.063	-0.810	1.00	14.10
ATOM	353	C	THR	150	0.223	12.129	-3.496	1.00	13.98
ATOM	354	O	THR	150	-0.137	11.087	-2.944	1.00	16.67
ATOM	355	N	ALA	151	-0.529	12.775	-4.386	1.00	13.39
ATOM	356	CA	ALA	151	-1.846	12.279	-4.766	1.00	11.01
ATOM	357	CB	ALA	151	-2.570	13.315	-5.629	1.00	12.89
ATOM	358	C	ALA	151	-1.716	10.959	-5.526	1.00	13.20
ATOM	359	O	ALA	151	-2.499	10.027	-5.307	1.00	12.07
ATOM	360	N	GLN	152	-0.728	10.883	-6.418	1.00	13.78
ATOM	361	CA	GLN	152	-0.501	9.669	-7.215	1.00	15.63

ATOM	362	CB	GLN	152	0.674	9.858	-8.183	1.00	18.69
ATOM	363	CG	GLN	152	0.727	11.204	-8.878	1.00	23.07
ATOM	364	CD	GLN	152	-0.188	11.297	-10.075	1.00	27.66
ATOM	365	OE1	GLN	152	-1.397	11.056	-9.976	1.00	31.28
ATOM	366	NE2	GLN	152	0.382	11.664	-11.223	1.00	28.87
ATOM	367	C	GLN	152	-0.159	8.524	-6.275	1.00	14.57
ATOM	368	O	GLN	152	-0.710	7.429	-6.379	1.00	16.88
ATOM	369	N	VAL	153	0.772	8.787	-5.365	1.00	11.76
ATOM	370	CA	VAL	153	1.208	7.795	-4.392	1.00	10.77
ATOM	371	CB	VAL	153	2.188	8.415	-3.382	1.00	12.54
ATOM	372	CG1	VAL	153	2.531	7.401	-2.284	1.00	11.39
ATOM	373	CG2	VAL	153	3.445	8.877	-4.113	1.00	13.70
ATOM	374	C	VAL	153	0.035	7.201	-3.627	1.00	9.29
ATOM	375	O	VAL	153	-0.064	5.977	-3.479	1.00	9.84
ATOM	376	N	ILE	154	-0.852	8.069	-3.149	1.00	7.89
ATOM	377	CA	ILE	154	-2.016	7.632	-2.394	1.00	9.24
ATOM	378	CB	ILE	154	-2.793	8.836	-1.802	1.00	6.77
ATOM	379	CG2	ILE	154	-4.020	8.346	-1.050	1.00	3.00
ATOM	380	CG1	ILE	154	-1.890	9.620	-0.837	1.00	7.16
ATOM	381	CD1	ILE	154	-2.479	10.960	-0.339	1.00	5.79
ATOM	382	C	ILE	154	-2.916	6.824	-3.318	1.00	10.47
ATOM	383	O	ILE	154	-3.350	5.736	-2.960	1.00	12.05
ATOM	384	N	ALA	155	-3.171	7.351	-4.515	1.00	12.23
ATOM	385	CA	ALA	155	-4.016	6.679	-5.506	1.00	13.49
ATOM	386	CB	ALA	155	-4.117	7.534	-6.774	1.00	14.88
ATOM	387	C	ALA	155	-3.506	5.284	-5.875	1.00	13.96
ATOM	388	O	ALA	155	-4.302	4.387	-6.168	1.00	12.79
ATOM	389	N	SER	156	-2.186	5.104	-5.873	1.00	13.52
ATOM	390	CA	SER	156	-1.599	3.816	-6.226	1.00	13.41
ATOM	391	CB	SER	156	-0.065	3.912	-6.283	1.00	12.71
ATOM	392	OG	SER	156	0.537	3.842	-4.999	1.00	11.43
ATOM	393	C	SER	156	-2.009	2.675	-5.293	1.00	14.50
ATOM	394	O	SER	156	-1.829	1.502	-5.634	1.00	15.94
ATOM	395	N	TYR	157	-2.553	3.001	-4.122	1.00	13.51
ATOM	396	CA	TYR	157	-2.990	1.953	-3.202	1.00	13.60
ATOM	397	CB	TYR	157	-3.032	2.463	-1.758	1.00	13.28
ATOM	398	CG	TYR	157	-1.659	2.635	-1.166	1.00	11.73
ATOM	399	CD1	TYR	157	-0.878	3.744	-1.479	1.00	11.85
ATOM	400	CE1	TYR	157	0.417	3.886	-0.971	1.00	10.97
ATOM	401	CD2	TYR	157	-1.116	1.661	-0.326	1.00	12.80
ATOM	402	CE2	TYR	157	0.175	1.788	0.186	1.00	12.30
ATOM	403	CZ	TYR	157	0.936	2.905	-0.142	1.00	12.80
ATOM	404	OH	TYR	157	2.221	3.020	0.355	1.00	13.77
ATOM	405	C	TYR	157	-4.356	1.405	-3.599	1.00	13.62
ATOM	406	O	TYR	157	-4.817	0.402	-3.057	1.00	14.03
ATOM	407	N	GLY	158	-4.997	2.066	-4.555	1.00	12.65
ATOM	408	CA	GLY	158	-6.296	1.610	-5.010	1.00	14.07
ATOM	409	C	GLY	158	-7.299	1.415	-3.890	1.00	14.14
ATOM	410	O	GLY	158	-7.426	2.267	-3.009	1.00	14.91
ATOM	411	N	SER	159	-8.001	0.284	-3.922	1.00	15.51
ATOM	412	CA	SER	159	-9.028	-0.041	-2.928	1.00	16.40
ATOM	413	CB	SER	159	-9.755	-1.331	-3.320	1.00	17.88
ATOM	414	OG	SER	159	-8.894	-2.460	-3.237	1.00	25.71
ATOM	415	C	SER	159	-8.554	-0.185	-1.486	1.00	14.65
ATOM	416	O	SER	159	-9.374	-0.197	-0.570	1.00	14.41
ATOM	417	N	ALA	160	-7.249	-0.304	-1.272	1.00	13.82
ATOM	418	CA	ALA	160	-6.739	-0.454	0.085	1.00	13.28
ATOM	419	CB	ALA	160	-5.228	-0.680	0.063	1.00	13.76
ATOM	420	C	ALA	160	-7.087	0.763	0.945	1.00	13.76
ATOM	421	O	ALA	160	-7.156	0.663	2.174	1.00	15.15
ATOM	422	N	VAL	161	-7.311	1.911	0.309	1.00	12.38
ATOM	423	CA	VAL	161	-7.662	3.112	1.059	1.00	12.29
ATOM	424	CB	VAL	161	-6.436	4.042	1.258	1.00	13.86
ATOM	425	CG1	VAL	161	-5.334	3.307	1.992	1.00	12.49
ATOM	426	CG2	VAL	161	-5.940	4.549	-0.104	1.00	12.62
ATOM	427	C	VAL	161	-8.740	3.925	0.367	1.00	13.24
ATOM	428	O	VAL	161	-9.092	3.665	-0.786	1.00	14.49

ATOM	429	N	THR	162	-9.269	4.907	1.093	1.00	12.97
ATOM	430	CA	THR	162	-10.269	5.813	0.565	1.00	13.31
ATOM	431	CB	THR	162	-11.530	5.878	1.466	1.00	12.73
ATOM	432	OG1	THR	162	-12.203	4.611	1.442	1.00	12.66
ATOM	433	CG2	THR	162	-12.492	6.962	0.963	1.00	13.71
ATOM	434	C	THR	162	-9.555	7.162	0.566	1.00	13.84
ATOM	435	O	THR	162	-9.174	7.671	1.623	1.00	12.78
ATOM	436	N	HIS	163	-9.366	7.727	-0.623	1.00	11.53
ATOM	437	CA	HIS	163	-8.666	8.995	-0.781	1.00	12.19
ATOM	438	CB	HIS	163	-7.783	8.917	-2.039	1.00	10.96
ATOM	439	CG	HIS	163	-6.853	10.076	-2.213	1.00	12.05
ATOM	440	CD2	HIS	163	-6.484	11.064	-1.363	1.00	12.44
ATOM	441	ND1	HIS	163	-6.164	10.305	-3.387	1.00	12.04
ATOM	442	CE1	HIS	163	-5.414	11.385	-3.253	1.00	9.88
ATOM	443	NE2	HIS	163	-5.591	11.865	-2.034	1.00	15.02
ATOM	444	C	HIS	163	-9.651	10.155	-0.909	1.00	11.18
ATOM	445	O	HIS	163	-10.449	10.184	-1.850	1.00	11.93
ATOM	446	N	ILE	164	-9.621	11.087	0.046	1.00	11.27
ATOM	447	CA	ILE	164	-10.492	12.258	-0.003	1.00	10.61
ATOM	448	CB	ILE	164	-11.498	12.304	1.192	1.00	10.27
ATOM	449	CG2	ILE	164	-12.421	11.093	1.115	1.00	8.30
ATOM	450	CG1	ILE	164	-10.756	12.357	2.529	1.00	10.16
ATOM	451	CD1	ILE	164	-11.673	12.546	3.737	1.00	10.55
ATOM	452	C	ILE	164	-9.620	13.509	-0.015	1.00	12.10
ATOM	453	O	ILE	164	-8.505	13.518	0.531	1.00	11.87
ATOM	454	N	ARG	165	-10.122	14.564	-0.644	1.00	11.87
ATOM	455	CA	ARG	165	-9.347	15.789	-0.776	1.00	13.13
ATOM	456	CB	ARG	165	-9.036	16.017	-2.255	1.00	13.85
ATOM	457	CG	ARG	165	-8.405	14.806	-2.914	1.00	15.69
ATOM	458	CD	ARG	165	-8.069	15.048	-4.375	1.00	22.37
ATOM	459	NE	ARG	165	-7.617	13.815	-5.019	1.00	25.63
ATOM	460	CZ	ARG	165	-6.930	13.764	-6.159	1.00	27.65
ATOM	461	NH1	ARG	165	-6.607	14.884	-6.795	1.00	27.98
ATOM	462	NH2	ARG	165	-6.560	12.591	-6.661	1.00	28.12
ATOM	463	C	ARG	165	-9.989	17.029	-0.192	1.00	12.50
ATOM	464	O	ARG	165	-11.112	17.395	-0.554	1.00	13.60
ATOM	465	N	GLN	166	-9.263	17.672	0.720	1.00	10.65
ATOM	466	CA	GLN	166	-9.730	18.890	1.356	1.00	10.92
ATOM	467	CB	GLN	166	-8.615	19.457	2.237	1.00	10.79
ATOM	468	CG	GLN	166	-9.084	20.383	3.346	1.00	11.11
ATOM	469	CD	GLN	166	-9.347	21.786	2.847	1.00	11.30
ATOM	470	OE1	GLN	166	-10.497	22.203	2.670	1.00	8.95
ATOM	471	NE2	GLN	166	-8.272	22.525	2.604	1.00	10.73
ATOM	472	C	GLN	166	-10.053	19.799	0.165	1.00	10.59
ATOM	473	O	GLN	166	-9.211	20.031	-0.695	1.00	7.16
ATOM	474	N	PRO	167	-11.290	20.310	0.098	1.00	11.35
ATOM	475	CD	PRO	167	-12.381	20.059	1.059	1.00	10.93
ATOM	476	CA	PRO	167	-11.743	21.174	-0.997	1.00	13.16
ATOM	477	CB	PRO	167	-13.260	21.046	-0.910	1.00	11.15
ATOM	478	CG	PRO	167	-13.481	20.994	0.572	1.00	12.32
ATOM	479	C	PRO	167	-11.302	22.631	-1.089	1.00	15.45
ATOM	480	O	PRO	167	-11.345	23.210	-2.173	1.00	19.39
ATOM	481	N	ASP	168	-10.873	23.229	0.018	1.00	16.01
ATOM	482	CA	ASP	168	-10.486	24.638	-0.001	1.00	16.48
ATOM	483	CB	ASP	168	-11.174	25.356	1.162	1.00	17.81
ATOM	484	CG	ASP	168	-11.098	26.859	1.042	1.00	20.10
ATOM	485	OD1	ASP	168	-10.636	27.339	-0.011	1.00	21.59
ATOM	486	OD2	ASP	168	-11.505	27.559	1.996	1.00	22.23
ATOM	487	C	ASP	168	-8.979	24.853	0.068	1.00	16.68
ATOM	488	O	ASP	168	-8.384	24.773	1.141	1.00	16.53
ATOM	489	N	LEU	169	-8.364	25.141	-1.075	1.00	17.45
ATOM	490	CA	LEU	169	-6.920	25.345	-1.121	1.00	18.41
ATOM	491	CB	LEU	169	-6.335	24.648	-2.353	1.00	18.24
ATOM	492	CG	LEU	169	-6.589	23.135	-2.360	1.00	20.62
ATOM	493	CD1	LEU	169	-5.843	22.482	-3.507	1.00	21.42
ATOM	494	CD2	LEU	169	-6.137	22.541	-1.030	1.00	19.66
ATOM	495	C	LEU	169	-6.480	26.804	-1.097	1.00	19.47

ATOM	496	O	LEU	169	-5.305	27.105	-1.304	1.00	20.15
ATOM	497	N	SER	170	-7.415	27.707	-0.832	1.00	18.24
ATOM	498	CA	SER	170	-7.100	29.131	-0.797	1.00	18.47
ATOM	499	CB	SER	170	-8.380	29.946	-0.607	1.00	18.55
ATOM	500	OG	SER	170	-8.904	29.737	0.693	1.00	18.73
ATOM	501	C	SER	170	-6.143	29.457	0.343	1.00	17.95
ATOM	502	O	SER	170	-6.017	28.692	1.296	1.00	17.26
ATOM	503	N	ASN	171	-5.460	30.594	0.243	1.00	17.82
ATOM	504	CA	ASN	171	-4.560	31.003	1.309	1.00	18.76
ATOM	505	CB	ASN	171	-3.607	32.107	0.849	1.00	21.01
ATOM	506	CG	ASN	171	-2.502	31.584	-0.045	1.00	23.36
ATOM	507	OD1	ASN	171	-1.950	30.505	0.195	1.00	24.21
ATOM	508	ND2	ASN	171	-2.160	32.351	-1.072	1.00	25.22
ATOM	509	C	ASN	171	-5.423	31.511	2.446	1.00	18.53
ATOM	510	O	ASN	171	-6.561	31.942	2.238	1.00	18.75
ATOM	511	N	ILE	172	-4.884	31.465	3.654	1.00	17.21
ATOM	512	CA	ILE	172	-5.636	31.901	4.810	1.00	17.15
ATOM	513	CB	ILE	172	-5.608	30.809	5.902	1.00	14.35
ATOM	514	CG2	ILE	172	-6.371	31.270	7.133	1.00	14.74
ATOM	515	CG1	ILE	172	-6.225	29.522	5.341	1.00	14.90
ATOM	516	CD1	ILE	172	-6.291	28.380	6.322	1.00	12.99
ATOM	517	C	ILE	172	-5.121	33.223	5.365	1.00	17.74
ATOM	518	O	ILE	172	-3.910	33.435	5.477	1.00	18.26
ATOM	519	N	ALA	173	-6.054	34.117	5.688	1.00	18.06
ATOM	520	CA	ALA	173	-5.710	35.421	6.241	1.00	18.43
ATOM	521	CB	ALA	173	-6.873	36.396	6.049	1.00	18.98
ATOM	522	C	ALA	173	-5.402	35.253	7.727	1.00	17.45
ATOM	523	O	ALA	173	-6.305	35.060	8.535	1.00	19.03
ATOM	524	N	VAL	174	-4.124	35.335	8.080	1.00	16.31
ATOM	525	CA	VAL	174	-3.702	35.175	9.464	1.00	13.65
ATOM	526	CB	VAL	174	-2.235	34.681	9.528	1.00	11.47
ATOM	527	CG1	VAL	174	-2.093	33.353	8.787	1.00	11.90
ATOM	528	CG2	VAL	174	-1.311	35.730	8.909	1.00	12.34
ATOM	529	C	VAL	174	-3.819	36.468	10.276	1.00	14.29
ATOM	530	O	VAL	174	-3.960	37.556	9.723	1.00	12.89
ATOM	531	N	GLN	175	-3.785	36.338	11.598	1.00	14.89
ATOM	532	CA	GLN	175	-3.851	37.505	12.459	1.00	14.87
ATOM	533	CB	GLN	175	-4.218	37.086	13.887	1.00	15.12
ATOM	534	CG	GLN	175	-5.704	36.772	14.055	1.00	15.29
ATOM	535	CD	GLN	175	-6.573	38.008	13.894	1.00	17.36
ATOM	536	OE1	GLN	175	-6.405	38.987	14.616	1.00	17.78
ATOM	537	NE2	GLN	175	-7.502	37.970	12.943	1.00	18.66
ATOM	538	C	GLN	175	-2.490	38.205	12.400	1.00	15.33
ATOM	539	O	GLN	175	-1.500	37.610	11.957	1.00	15.49
ATOM	540	N	PRO	176	-2.423	39.476	12.837	1.00	15.05
ATOM	541	CD	PRO	176	-3.517	40.237	13.462	1.00	15.32
ATOM	542	CA	PRO	176	-1.187	40.272	12.826	1.00	16.16
ATOM	543	CB	PRO	176	-1.592	41.555	13.552	1.00	15.28
ATOM	544	CG	PRO	176	-3.055	41.660	13.268	1.00	15.95
ATOM	545	C	PRO	176	0.041	39.631	13.458	1.00	16.04
ATOM	546	O	PRO	176	1.167	39.966	13.102	1.00	17.89
ATOM	547	N	ASP	177	-0.169	38.714	14.394	1.00	16.81
ATOM	548	CA	ASP	177	0.943	38.061	15.079	1.00	16.04
ATOM	549	CB	ASP	177	0.573	37.851	16.557	1.00	15.39
ATOM	550	CG	ASP	177	-0.663	36.967	16.747	1.00	16.70
ATOM	551	OD1	ASP	177	-1.598	37.026	15.910	1.00	16.88
ATOM	552	OD2	ASP	177	-0.709	36.221	17.755	1.00	15.17
ATOM	553	C	ASP	177	1.378	36.729	14.467	1.00	16.92
ATOM	554	O	ASP	177	2.333	36.112	14.938	1.00	15.81
ATOM	555	N	HIS	178	0.713	36.307	13.395	1.00	15.81
ATOM	556	CA	HIS	178	1.007	35.007	12.793	1.00	13.63
ATOM	557	CB	HIS	178	-0.230	34.121	12.936	1.00	13.76
ATOM	558	CG	HIS	178	-0.593	33.815	14.359	1.00	12.41
ATOM	559	CD2	HIS	178	0.171	33.715	15.472	1.00	10.30
ATOM	560	ND1	HIS	178	-1.878	33.501	14.747	1.00	11.11
ATOM	561	CE1	HIS	178	-1.889	33.219	16.038	1.00	13.44
ATOM	562	NE2	HIS	178	-0.659	33.341	16.501	1.00	13.56

ATOM	563	C	HIS	178	1.484	34.970	11.344	1.00	13.75
ATOM	564	O	HIS	178	1.270	33.979	10.644	1.00	11.54
ATOM	565	N	ARG	179	2.149	36.026	10.900	1.00	13.02
ATOM	566	CA	ARG	179	2.643	36.084	9.525	1.00	16.44
ATOM	567	CB	ARG	179	3.498	37.340	9.327	1.00	19.44
ATOM	568	CG	ARG	179	3.178	38.115	8.055	1.00	26.52
ATOM	569	CD	ARG	179	1.805	38.793	8.120	1.00	28.90
ATOM	570	NE	ARG	179	1.765	39.886	9.095	1.00	31.02
ATOM	571	CZ	ARG	179	0.710	40.677	9.291	1.00	31.06
ATOM	572	NH1	ARG	179	-0.398	40.500	8.582	1.00	29.73
ATOM	573	NH2	ARG	179	0.762	41.647	10.195	1.00	29.44
ATOM	574	C	ARG	179	3.467	34.844	9.177	1.00	16.06
ATOM	575	O	ARG	179	3.351	34.285	8.082	1.00	15.24
ATOM	576	N	LYS	180	4.290	34.408	10.119	1.00	15.25
ATOM	577	CA	LYS	180	5.142	33.250	9.900	1.00	17.11
ATOM	578	CB	LYS	180	6.422	33.386	10.737	1.00	17.31
ATOM	579	CG	LYS	180	7.126	34.730	10.559	1.00	20.60
ATOM	580	CD	LYS	180	8.545	34.744	11.119	1.00	23.05
ATOM	581	CE	LYS	180	8.585	34.487	12.616	1.00	24.27
ATOM	582	NZ	LYS	180	8.167	33.095	12.936	1.00	24.99
ATOM	583	C	LYS	180	4.478	31.909	10.213	1.00	16.54
ATOM	584	O	LYS	180	5.123	30.870	10.126	1.00	18.10
ATOM	585	N	PHE	181	3.191	31.909	10.541	1.00	16.34
ATOM	586	CA	PHE	181	2.548	30.650	10.899	1.00	15.72
ATOM	587	CB	PHE	181	2.210	30.659	12.391	1.00	16.77
ATOM	588	CG	PHE	181	3.373	31.015	13.274	1.00	18.24
ATOM	589	CD1	PHE	181	3.568	32.327	13.696	1.00	19.04
ATOM	590	CD2	PHE	181	4.287	30.043	13.668	1.00	19.05
ATOM	591	CE1	PHE	181	4.655	32.665	14.496	1.00	18.67
ATOM	592	CE2	PHE	181	5.379	30.373	14.468	1.00	18.62
ATOM	593	CZ	PHE	181	5.561	31.687	14.881	1.00	18.99
ATOM	594	C	PHE	181	1.307	30.243	10.115	1.00	16.33
ATOM	595	O	PHE	181	0.427	29.588	10.664	1.00	14.41
ATOM	596	N	GLN	182	1.230	30.604	8.837	1.00	17.25
ATOM	597	CA	GLN	182	0.058	30.235	8.060	1.00	18.13
ATOM	598	CB	GLN	182	0.096	30.875	6.670	1.00	19.04
ATOM	599	CG	GLN	182	-1.188	30.629	5.889	1.00	22.51
ATOM	600	CD	GLN	182	-1.335	31.530	4.688	1.00	24.33
ATOM	601	OE1	GLN	182	-2.280	31.394	3.915	1.00	28.47
ATOM	602	NE2	GLN	182	-0.403	32.465	4.525	1.00	25.56
ATOM	603	C	GLN	182	-0.069	28.718	7.932	1.00	17.26
ATOM	604	O	GLN	182	-1.173	28.194	7.787	1.00	17.25
ATOM	605	N	GLY	183	1.059	28.012	7.979	1.00	16.36
ATOM	606	CA	GLY	183	1.013	26.565	7.880	1.00	16.03
ATOM	607	C	GLY	183	0.130	25.971	8.962	1.00	15.37
ATOM	608	O	GLY	183	-0.615	25.020	8.716	1.00	16.30
ATOM	609	N	TYR	184	0.209	26.530	10.168	1.00	15.63
ATOM	610	CA	TYR	184	-0.605	26.040	11.282	1.00	12.82
ATOM	611	CB	TYR	184	-0.152	26.676	12.595	1.00	12.50
ATOM	612	CG	TYR	184	1.261	26.298	12.954	1.00	13.85
ATOM	613	CD1	TYR	184	2.332	27.122	12.617	1.00	14.55
ATOM	614	CE1	TYR	184	3.647	26.743	12.887	1.00	17.00
ATOM	615	CD2	TYR	184	1.534	25.083	13.574	1.00	14.97
ATOM	616	CE2	TYR	184	2.845	24.688	13.845	1.00	17.91
ATOM	617	CZ	TYR	184	3.895	25.524	13.498	1.00	18.43
ATOM	618	OH	TYR	184	5.190	25.135	13.755	1.00	20.05
ATOM	619	C	TYR	184	-2.094	26.296	11.060	1.00	12.14
ATOM	620	O	TYR	184	-2.936	25.537	11.547	1.00	12.20
ATOM	621	N	TYR	185	-2.417	27.367	10.336	1.00	10.53
ATOM	622	CA	TYR	185	-3.809	27.689	10.045	1.00	10.55
ATOM	623	CB	TYR	185	-3.932	29.075	9.396	1.00	9.30
ATOM	624	CG	TYR	185	-3.908	30.244	10.361	1.00	9.37
ATOM	625	CD1	TYR	185	-2.768	30.538	11.116	1.00	8.53
ATOM	626	CE1	TYR	185	-2.745	31.628	11.986	1.00	8.23
ATOM	627	CD2	TYR	185	-5.027	31.069	10.503	1.00	8.29
ATOM	628	CE2	TYR	185	-5.013	32.158	11.368	1.00	7.75
ATOM	629	CZ	TYR	185	-3.871	32.430	12.106	1.00	6.66

ATOM	630	OH	TYR	185	-3.871	33.495	12.974	1.00	7.11
ATOM	631	C	TYR	185	-4.338	26.635	9.073	1.00	12.31
ATOM	632	O	TYR	185	-5.486	26.188	9.177	1.00	15.20
ATOM	633	N	LYS	186	-3.493	26.247	8.121	1.00	12.42
ATOM	634	CA	LYS	186	-3.876	25.252	7.131	1.00	11.01
ATOM	635	CB	LYS	186	-2.810	25.181	6.026	1.00	13.10
ATOM	636	CG	LYS	186	-2.702	26.499	5.252	1.00	16.96
ATOM	637	CD	LYS	186	-1.834	26.405	4.011	1.00	19.58
ATOM	638	CE	LYS	186	-1.888	27.719	3.234	1.00	22.94
ATOM	639	NZ	LYS	186	-1.120	27.679	1.961	1.00	24.21
ATOM	640	C	LYS	186	-4.090	23.893	7.790	1.00	10.16
ATOM	641	O	LYS	186	-5.026	23.167	7.435	1.00	9.33
ATOM	642	N	ILE	187	-3.245	23.560	8.770	1.00	10.54
ATOM	643	CA	ILE	187	-3.370	22.287	9.476	1.00	10.47
ATOM	644	CB	ILE	187	-2.221	22.077	10.507	1.00	9.82
ATOM	645	CG2	ILE	187	-2.499	20.844	11.357	1.00	13.47
ATOM	646	CG1	ILE	187	-0.882	21.924	9.778	1.00	11.99
ATOM	647	CD1	ILE	187	0.324	21.800	10.704	1.00	12.20
ATOM	648	C	ILE	187	-4.707	22.231	10.217	1.00	9.63
ATOM	649	O	ILE	187	-5.441	21.243	10.120	1.00	8.68
ATOM	650	N	ALA	188	-5.032	23.292	10.950	1.00	10.22
ATOM	651	CA	ALA	188	-6.288	23.315	11.691	1.00	10.25
ATOM	652	CB	ALA	188	-6.390	24.595	12.507	1.00	9.59
ATOM	653	C	ALA	188	-7.477	23.185	10.747	1.00	10.89
ATOM	654	O	ALA	188	-8.369	22.362	10.971	1.00	11.02
ATOM	655	N	ARG	189	-7.489	23.990	9.684	1.00	9.54
ATOM	656	CA	ARG	189	-8.576	23.933	8.708	1.00	9.53
ATOM	657	CB	ARG	189	-8.326	24.892	7.537	1.00	10.47
ATOM	658	CG	ARG	189	-9.297	24.678	6.376	1.00	8.84
ATOM	659	CD	ARG	189	-9.107	25.729	5.288	1.00	9.04
ATOM	660	NE	ARG	189	-7.833	25.573	4.593	1.00	10.98
ATOM	661	CZ	ARG	189	-7.383	26.418	3.674	1.00	9.49
ATOM	662	NH1	ARG	189	-8.107	27.480	3.345	1.00	11.30
ATOM	663	NH2	ARG	189	-6.219	26.198	3.079	1.00	7.44
ATOM	664	C	ARG	189	-8.745	22.521	8.163	1.00	9.57
ATOM	665	O	ARG	189	-9.874	22.033	8.042	1.00	11.18
ATOM	666	N	HIS	190	-7.634	21.858	7.832	1.00	8.44
ATOM	667	CA	HIS	190	-7.710	20.495	7.307	1.00	8.46
ATOM	668	CB	HIS	190	-6.336	19.981	6.864	1.00	9.39
ATOM	669	CG	HIS	190	-6.393	18.664	6.150	1.00	8.35
ATOM	670	CD2	HIS	190	-7.436	17.987	5.609	1.00	9.30
ATOM	671	ND1	HIS	190	-5.272	17.904	5.893	1.00	8.82
ATOM	672	CE1	HIS	190	-5.620	16.817	5.226	1.00	9.58
ATOM	673	NE2	HIS	190	-6.928	16.843	5.040	1.00	9.23
ATOM	674	C	HIS	190	-8.288	19.538	8.343	1.00	8.88
ATOM	675	O	HIS	190	-9.161	18.725	8.020	1.00	9.00
ATOM	676	N	TYR	191	-7.800	19.615	9.580	1.00	6.85
ATOM	677	CA	TYR	191	-8.319	18.753	10.637	1.00	9.06
ATOM	678	CB	TYR	191	-7.656	19.062	11.982	1.00	9.14
ATOM	679	CG	TYR	191	-6.465	18.191	12.272	1.00	7.88
ATOM	680	CD1	TYR	191	-5.306	18.287	11.502	1.00	6.83
ATOM	681	CE1	TYR	191	-4.203	17.487	11.767	1.00	9.37
ATOM	682	CD2	TYR	191	-6.494	17.269	13.321	1.00	6.45
ATOM	683	CE2	TYR	191	-5.399	16.465	13.598	1.00	8.49
ATOM	684	CZ	TYR	191	-4.255	16.576	12.817	1.00	8.71
ATOM	685	OH	TYR	191	-3.170	15.768	13.077	1.00	9.63
ATOM	686	C	TYR	191	-9.823	18.915	10.785	1.00	9.84
ATOM	687	O	TYR	191	-10.550	17.929	10.918	1.00	7.17
ATOM	688	N	ARG	192	-10.302	20.155	10.760	1.00	11.35
ATOM	689	CA	ARG	192	-11.736	20.361	10.900	1.00	11.81
ATOM	690	CB	ARG	192	-12.087	21.849	10.921	1.00	17.23
ATOM	691	CG	ARG	192	-13.587	22.085	11.027	1.00	21.28
ATOM	692	CD	ARG	192	-13.965	23.551	10.990	1.00	27.35
ATOM	693	NE	ARG	192	-14.047	24.141	12.324	1.00	32.19
ATOM	694	CZ	ARG	192	-14.715	25.259	12.600	1.00	33.87
ATOM	695	NH1	ARG	192	-15.357	25.900	11.631	1.00	34.07
ATOM	696	NH2	ARG	192	-14.747	25.736	13.841	1.00	33.34

ATOM	697	C	ARG	192	-12.490	19.671	9.766	1.00	11.58
ATOM	698	O	ARG	192	-13.444	18.944	10.005	1.00	9.22
ATOM	699	N	TRP	193	-12.058	19.888	8.529	1.00	11.60
ATOM	700	CA	TRP	193	-12.727	19.265	7.397	1.00	12.68
ATOM	701	CB	TRP	193	-12.147	19.775	6.069	1.00	10.74
ATOM	702	CG	TRP	193	-12.882	19.222	4.876	1.00	11.01
ATOM	703	CD2	TRP	193	-12.532	18.058	4.117	1.00	11.46
ATOM	704	CE2	TRP	193	-13.536	17.880	3.135	1.00	11.14
ATOM	705	CE3	TRP	193	-11.470	17.147	4.172	1.00	9.60
ATOM	706	CD1	TRP	193	-14.050	19.689	4.339	1.00	12.46
ATOM	707	NE1	TRP	193	-14.448	18.888	3.293	1.00	12.85
ATOM	708	CZ2	TRP	193	-13.508	16.826	2.212	1.00	11.74
ATOM	709	CZ3	TRP	193	-11.440	16.096	3.251	1.00	10.42
ATOM	710	CH2	TRP	193	-12.455	15.948	2.284	1.00	12.95
ATOM	711	C	TRP	193	-12.628	17.737	7.431	1.00	13.18
ATOM	712	O	TRP	193	-13.637	17.038	7.256	1.00	13.02
ATOM	713	N	ALA	194	-11.418	17.224	7.660	1.00	12.50
ATOM	714	CA	ALA	194	-11.181	15.779	7.696	1.00	11.15
ATOM	715	CB	ALA	194	-9.689	15.494	7.876	1.00	11.03
ATOM	716	C	ALA	194	-11.977	15.083	8.791	1.00	11.89
ATOM	717	O	ALA	194	-12.606	14.054	8.546	1.00	12.53
ATOM	718	N	LEU	195	-11.947	15.631	10.002	1.00	10.20
ATOM	719	CA	LEU	195	-12.696	15.018	11.090	1.00	11.79
ATOM	720	CB	LEU	195	-12.316	15.668	12.424	1.00	10.87
ATOM	721	CG	LEU	195	-10.888	15.315	12.864	1.00	10.64
ATOM	722	CD1	LEU	195	-10.483	16.140	14.053	1.00	11.96
ATOM	723	CD2	LEU	195	-10.809	13.830	13.186	1.00	12.40
ATOM	724	C	LEU	195	-14.202	15.117	10.828	1.00	10.09
ATOM	725	O	LEU	195	-14.955	14.211	11.176	1.00	11.46
ATOM	726	N	GLY	196	-14.627	16.208	10.196	1.00	9.97
ATOM	727	CA	GLY	196	-16.035	16.381	9.880	1.00	9.42
ATOM	728	C	GLY	196	-16.492	15.336	8.877	1.00	10.26
ATOM	729	O	GLY	196	-17.641	14.899	8.902	1.00	9.53
ATOM	730	N	GLN	197	-15.594	14.937	7.982	1.00	10.86
ATOM	731	CA	GLN	197	-15.913	13.924	6.983	1.00	13.26
ATOM	732	CB	GLN	197	-14.778	13.819	5.953	1.00	14.20
ATOM	733	CG	GLN	197	-14.678	14.996	4.983	1.00	18.00
ATOM	734	CD	GLN	197	-15.884	15.102	4.058	1.00	20.43
ATOM	735	OE1	GLN	197	-16.201	14.164	3.326	1.00	22.88
ATOM	736	NE2	GLN	197	-16.559	16.248	4.087	1.00	22.29
ATOM	737	C	GLN	197	-16.124	12.563	7.652	1.00	12.76
ATOM	738	O	GLN	197	-17.068	11.839	7.337	1.00	13.06
ATOM	739	N	ILE	198	-15.229	12.227	8.574	1.00	11.42
ATOM	740	CA	ILE	198	-15.279	10.960	9.293	1.00	10.34
ATOM	741	CB	ILE	198	-13.966	10.779	10.149	1.00	12.72
ATOM	742	CG2	ILE	198	-14.312	10.514	11.597	1.00	13.45
ATOM	743	CG1	ILE	198	-13.128	9.598	9.635	1.00	13.66
ATOM	744	CD1	ILE	198	-12.784	9.639	8.150	1.00	15.66
ATOM	745	C	ILE	198	-16.521	10.847	10.191	1.00	11.01
ATOM	746	O	ILE	198	-17.164	9.794	10.249	1.00	10.50
ATOM	747	N	PHE	199	-16.872	11.931	10.880	1.00	9.85
ATOM	748	CA	PHE	199	-18.016	11.898	11.789	1.00	12.52
ATOM	749	CB	PHE	199	-17.683	12.668	13.072	1.00	11.87
ATOM	750	CG	PHE	199	-16.510	12.106	13.831	1.00	11.32
ATOM	751	CD1	PHE	199	-15.330	12.825	13.939	1.00	11.29
ATOM	752	CD2	PHE	199	-16.586	10.851	14.435	1.00	13.61
ATOM	753	CE1	PHE	199	-14.237	12.313	14.641	1.00	11.50
ATOM	754	CE2	PHE	199	-15.494	10.325	15.140	1.00	11.99
ATOM	755	CZ	PHE	199	-14.319	11.061	15.243	1.00	13.30
ATOM	756	C	PHE	199	-19.362	12.384	11.244	1.00	14.10
ATOM	757	O	PHE	199	-20.407	12.025	11.790	1.00	14.81
ATOM	758	N	HIS	200	-19.349	13.185	10.181	1.00	13.88
ATOM	759	CA	HIS	200	-20.594	13.691	9.605	1.00	15.96
ATOM	760	CB	HIS	200	-20.501	15.195	9.324	1.00	16.05
ATOM	761	CG	HIS	200	-20.317	16.032	10.550	1.00	16.55
ATOM	762	CD2	HIS	200	-19.503	17.086	10.796	1.00	12.92
ATOM	763	ND1	HIS	200	-21.034	15.820	11.710	1.00	15.37

ATOM	764	CE1	HIS	200	-20.667	16.707	12.619	1.00	14.89
ATOM	765	NE2	HIS	200	-19.740	17.486	12.089	1.00	16.70
ATOM	766	C	HIS	200	-20.972	12.982	8.315	1.00	18.11
ATOM	767	O	HIS	200	-22.139	12.681	8.086	1.00	19.95
ATOM	768	N	ASN	201	-19.987	12.724	7.465	1.00	18.58
ATOM	769	CA	ASN	201	-20.252	12.061	6.201	1.00	19.43
ATOM	770	CB	ASN	201	-19.254	12.543	5.152	1.00	20.95
ATOM	771	CG	ASN	201	-19.348	14.038	4.921	1.00	25.05
ATOM	772	OD1	ASN	201	-20.261	14.519	4.248	1.00	26.97
ATOM	773	ND2	ASN	201	-18.414	14.786	5.495	1.00	28.26
ATOM	774	C	ASN	201	-20.204	10.548	6.348	1.00	19.23
ATOM	775	O	ASN	201	-21.217	9.875	6.141	1.00	19.59
ATOM	776	N	PHE	202	-19.043	10.006	6.707	1.00	17.05
ATOM	777	CA	PHE	202	-18.935	8.564	6.878	1.00	16.71
ATOM	778	CB	PHE	202	-17.471	8.137	7.017	1.00	17.72
ATOM	779	CG	PHE	202	-16.654	8.360	5.770	1.00	18.02
ATOM	780	CD1	PHE	202	-15.978	9.556	5.566	1.00	17.66
ATOM	781	CD2	PHE	202	-16.575	7.373	4.790	1.00	19.11
ATOM	782	CE1	PHE	202	-15.231	9.771	4.404	1.00	17.35
ATOM	783	CE2	PHE	202	-15.831	7.577	3.625	1.00	18.71
ATOM	784	CZ	PHE	202	-15.159	8.779	3.433	1.00	17.13
ATOM	785	C	PHE	202	-19.736	8.125	8.099	1.00	16.80
ATOM	786	O	PHE	202	-20.216	6.990	8.160	1.00	15.19
ATOM	787	N	ASN	203	-19.871	9.029	9.065	1.00	14.55
ATOM	788	CA	ASN	203	-20.640	8.775	10.283	1.00	17.07
ATOM	789	CB	ASN	203	-22.099	8.474	9.908	1.00	20.44
ATOM	790	CG	ASN	203	-23.045	8.555	11.097	1.00	25.36
ATOM	791	OD1	ASN	203	-24.173	8.061	11.036	1.00	29.01
ATOM	792	ND2	ASN	203	-22.597	9.188	12.181	1.00	24.85
ATOM	793	C	ASN	203	-20.084	7.647	11.161	1.00	15.89
ATOM	794	O	ASN	203	-20.828	6.780	11.620	1.00	16.33
ATOM	795	N	TYR	204	-18.776	7.667	11.394	1.00	15.66
ATOM	796	CA	TYR	204	-18.126	6.661	12.229	1.00	14.83
ATOM	797	CB	TYR	204	-16.644	6.549	11.862	1.00	16.17
ATOM	798	CG	TYR	204	-16.386	5.844	10.547	1.00	16.40
ATOM	799	CD1	TYR	204	-15.733	6.491	9.495	1.00	17.22
ATOM	800	CE1	TYR	204	-15.469	5.828	8.293	1.00	17.26
ATOM	801	CD2	TYR	204	-16.774	4.517	10.361	1.00	18.35
ATOM	802	CE2	TYR	204	-16.516	3.849	9.163	1.00	17.96
ATOM	803	CZ	TYR	204	-15.865	4.504	8.139	1.00	17.98
ATOM	804	OH	TYR	204	-15.597	3.826	6.973	1.00	21.54
ATOM	805	C	TYR	204	-18.279	7.054	13.695	1.00	14.42
ATOM	806	O	TYR	204	-18.357	8.237	14.019	1.00	13.64
ATOM	807	N	PRO	205	-18.304	6.064	14.604	1.00	13.88
ATOM	808	CD	PRO	205	-18.163	4.616	14.350	1.00	13.49
ATOM	809	CA	PRO	205	-18.458	6.323	16.038	1.00	13.22
ATOM	810	CB	PRO	205	-18.907	4.975	16.568	1.00	11.77
ATOM	811	CG	PRO	205	-18.049	4.038	15.766	1.00	13.06
ATOM	812	C	PRO	205	-17.188	6.809	16.724	1.00	11.71
ATOM	813	O	PRO	205	-17.227	7.278	17.862	1.00	10.13
ATOM	814	N	ALA	206	-16.064	6.690	16.025	1.00	11.36
ATOM	815	CA	ALA	206	-14.775	7.094	16.567	1.00	11.54
ATOM	816	CB	ALA	206	-14.369	6.143	17.693	1.00	11.71
ATOM	817	C	ALA	206	-13.749	7.051	15.444	1.00	11.90
ATOM	818	O	ALA	206	-14.071	6.644	14.323	1.00	13.95
ATOM	819	N	ALA	207	-12.521	7.478	15.734	1.00	12.75
ATOM	820	CA	ALA	207	-11.460	7.463	14.731	1.00	11.14
ATOM	821	CB	ALA	207	-11.697	8.574	13.719	1.00	12.19
ATOM	822	C	ALA	207	-10.056	7.600	15.326	1.00	12.50
ATOM	823	O	ALA	207	-9.859	8.223	16.375	1.00	10.74
ATOM	824	N	VAL	208	-9.078	6.998	14.656	1.00	12.35
ATOM	825	CA	VAL	208	-7.693	7.093	15.091	1.00	9.86
ATOM	826	CB	VAL	208	-6.997	5.706	15.113	1.00	12.26
ATOM	827	CG1	VAL	208	-5.498	5.866	15.410	1.00	7.21
ATOM	828	CG2	VAL	208	-7.639	4.822	16.194	1.00	9.28
ATOM	829	C	VAL	208	-7.011	8.018	14.083	1.00	10.30
ATOM	830	O	VAL	208	-6.897	7.692	12.899	1.00	10.07

ATOM	831	N	VAL	209	-6.584	9.180	14.566	1.00	9.11
ATOM	832	CA	VAL	209	-5.922	10.187	13.739	1.00	10.13
ATOM	833	CB	VAL	209	-6.099	11.609	14.346	1.00	10.24
ATOM	834	CG1	VAL	209	-5.557	12.654	13.384	1.00	8.23
ATOM	835	CG2	VAL	209	-7.572	11.879	14.660	1.00	8.21
ATOM	836	C	VAL	209	-4.421	9.888	13.643	1.00	11.76
ATOM	837	O	VAL	209	-3.730	9.809	14.663	1.00	11.66
ATOM	838	N	VAL	210	-3.925	9.747	12.417	1.00	11.15
ATOM	839	CA	VAL	210	-2.513	9.447	12.178	1.00	9.20
ATOM	840	CB	VAL	210	-2.331	7.992	11.691	1.00	10.51
ATOM	841	CG1	VAL	210	-0.855	7.703	11.480	1.00	10.51
ATOM	842	CG2	VAL	210	-2.938	7.019	12.701	1.00	9.73
ATOM	843	C	VAL	210	-1.919	10.368	11.116	1.00	9.32
ATOM	844	O	VAL	210	-2.347	10.349	9.965	1.00	7.67
ATOM	845	N	GLU	211	-0.929	11.172	11.488	1.00	8.01
ATOM	846	CA	GLU	211	-0.327	12.061	10.505	1.00	10.01
ATOM	847	CB	GLU	211	0.395	13.210	11.209	1.00	9.15
ATOM	848	CG	GLU	211	-0.580	14.011	12.063	1.00	13.09
ATOM	849	CD	GLU	211	0.024	15.253	12.662	1.00	13.74
ATOM	850	OE1	GLU	211	1.196	15.196	13.085	1.00	12.33
ATOM	851	OE2	GLU	211	-0.683	16.284	12.723	1.00	15.09
ATOM	852	C	GLU	211	0.599	11.279	9.570	1.00	10.13
ATOM	853	O	GLU	211	1.179	10.261	9.957	1.00	10.41
ATOM	854	N	ASP	212	0.714	11.762	8.337	1.00	9.51
ATOM	855	CA	ASP	212	1.510	11.116	7.295	1.00	9.70
ATOM	856	CB	ASP	212	1.456	11.957	6.015	1.00	10.24
ATOM	857	CG	ASP	212	2.137	13.304	6.178	1.00	9.59
ATOM	858	OD1	ASP	212	1.888	13.967	7.200	1.00	14.23
ATOM	859	OD2	ASP	212	2.914	13.705	5.288	1.00	14.29
ATOM	860	C	ASP	212	2.964	10.798	7.618	1.00	11.01
ATOM	861	O	ASP	212	3.581	9.986	6.921	1.00	10.95
ATOM	862	N	ASP	213	3.524	11.416	8.657	1.00	11.11
ATOM	863	CA	ASP	213	4.918	11.151	8.993	1.00	10.40
ATOM	864	CB	ASP	213	5.696	12.473	9.133	1.00	12.73
ATOM	865	CG	ASP	213	5.138	13.389	10.212	1.00	13.79
ATOM	866	OD1	ASP	213	4.046	13.104	10.751	1.00	10.99
ATOM	867	OD2	ASP	213	5.801	14.413	10.518	1.00	13.82
ATOM	868	C	ASP	213	5.113	10.264	10.224	1.00	9.85
ATOM	869	O	ASP	213	6.152	10.313	10.893	1.00	9.38
ATOM	870	N	LEU	214	4.119	9.431	10.508	1.00	8.38
ATOM	871	CA	LEU	214	4.211	8.526	11.646	1.00	8.22
ATOM	872	CB	LEU	214	3.030	8.715	12.607	1.00	8.79
ATOM	873	CG	LEU	214	2.728	10.115	13.156	1.00	10.50
ATOM	874	CD1	LEU	214	1.574	10.010	14.158	1.00	9.35
ATOM	875	CD2	LEU	214	3.966	10.701	13.825	1.00	7.37
ATOM	876	C	LEU	214	4.223	7.080	11.183	1.00	8.30
ATOM	877	O	LEU	214	3.470	6.693	10.280	1.00	9.71
ATOM	878	N	GLU	215	5.093	6.282	11.787	1.00	9.28
ATOM	879	CA	GLU	215	5.137	4.862	11.477	1.00	9.68
ATOM	880	CB	GLU	215	6.569	4.380	11.295	1.00	12.93
ATOM	881	CG	GLU	215	6.632	2.916	10.925	1.00	17.15
ATOM	882	CD	GLU	215	8.042	2.438	10.640	1.00	19.10
ATOM	883	OE1	GLU	215	8.769	3.145	9.907	1.00	19.26
ATOM	884	OE2	GLU	215	8.408	1.350	11.140	1.00	20.33
ATOM	885	C	GLU	215	4.516	4.167	12.685	1.00	10.33
ATOM	886	O	GLU	215	4.903	4.443	13.822	1.00	11.10
ATOM	887	N	VAL	216	3.555	3.279	12.448	1.00	9.51
ATOM	888	CA	VAL	216	2.894	2.568	13.542	1.00	9.71
ATOM	889	CB	VAL	216	1.444	2.187	13.163	1.00	9.47
ATOM	890	CG1	VAL	216	0.631	3.445	12.843	1.00	9.86
ATOM	891	CG2	VAL	216	1.455	1.243	11.964	1.00	9.95
ATOM	892	C	VAL	216	3.622	1.292	13.969	1.00	10.93
ATOM	893	O	VAL	216	4.289	0.640	13.165	1.00	10.14
ATOM	894	N	ALA	217	3.488	0.947	15.249	1.00	9.76
ATOM	895	CA	ALA	217	4.093	-0.258	15.806	1.00	10.00
ATOM	896	CB	ALA	217	4.154	-0.142	17.325	1.00	10.50
ATOM	897	C	ALA	217	3.242	-1.467	15.408	1.00	10.04

ATOM	898	O	ALA	217	2.092	-1.310	15.011	1.00	9.00
ATOM	899	N	PRO	218	3.795	-2.691	15.527	1.00	9.92
ATOM	900	CD	PRO	218	5.186	-2.971	15.935	1.00	11.27
ATOM	901	CA	PRO	218	3.093	-3.935	15.183	1.00	9.98
ATOM	902	CB	PRO	218	4.094	-5.020	15.591	1.00	8.72
ATOM	903	CG	PRO	218	5.422	-4.352	15.378	1.00	12.74
ATOM	904	C	PRO	218	1.755	-4.107	15.905	1.00	10.11
ATOM	905	O	PRO	218	0.799	-4.661	15.347	1.00	11.49
ATOM	906	N	ASP	219	1.694	-3.655	17.154	1.00	9.89
ATOM	907	CA	ASP	219	0.472	-3.779	17.931	1.00	10.68
ATOM	908	CB	ASP	219	0.782	-4.276	19.358	1.00	9.51
ATOM	909	CG	ASP	219	1.878	-3.474	20.051	1.00	10.70
ATOM	910	OD1	ASP	219	2.332	-2.444	19.509	1.00	9.65
ATOM	911	OD2	ASP	219	2.282	-3.881	21.163	1.00	11.17
ATOM	912	C	ASP	219	-0.322	-2.479	17.990	1.00	10.21
ATOM	913	O	ASP	219	-1.045	-2.224	18.947	1.00	10.79
ATOM	914	N	PHE	220	-0.192	-1.666	16.950	1.00	11.46
ATOM	915	CA	PHE	220	-0.902	-0.393	16.862	1.00	10.34
ATOM	916	CB	PHE	220	-0.540	0.298	15.542	1.00	11.72
ATOM	917	CG	PHE	220	-1.299	1.577	15.284	1.00	10.80
ATOM	918	CD1	PHE	220	-0.891	2.780	15.863	1.00	9.90
ATOM	919	CD2	PHE	220	-2.409	1.579	14.443	1.00	9.84
ATOM	920	CE1	PHE	220	-1.575	3.967	15.605	1.00	9.96
ATOM	921	CE2	PHE	220	-3.104	2.761	14.175	1.00	9.47
ATOM	922	CZ	PHE	220	-2.684	3.964	14.760	1.00	8.03
ATOM	923	C	PHE	220	-2.419	-0.587	16.942	1.00	10.32
ATOM	924	O	PHE	220	-3.081	0.032	17.772	1.00	10.53
ATOM	925	N	PHE	221	-2.966	-1.440	16.076	1.00	10.50
ATOM	926	CA	PHE	221	-4.405	-1.686	16.052	1.00	8.87
ATOM	927	CB	PHE	221	-4.790	-2.470	14.792	1.00	9.72
ATOM	928	CG	PHE	221	-4.313	-1.844	13.512	1.00	7.49
ATOM	929	CD1	PHE	221	-3.011	-2.064	13.054	1.00	6.99
ATOM	930	CD2	PHE	221	-5.167	-1.049	12.757	1.00	9.47
ATOM	931	CE1	PHE	221	-2.570	-1.498	11.853	1.00	8.01
ATOM	932	CE2	PHE	221	-4.741	-0.479	11.555	1.00	7.93
ATOM	933	CZ	PHE	221	-3.437	-0.706	11.102	1.00	8.73
ATOM	934	C	PHE	221	-4.872	-2.454	17.288	1.00	9.51
ATOM	935	O	PHE	221	-5.901	-2.126	17.884	1.00	10.03
ATOM	936	N	GLU	222	-4.120	-3.487	17.654	1.00	9.57
ATOM	937	CA	GLU	222	-4.421	-4.298	18.825	1.00	9.07
ATOM	938	CB	GLU	222	-3.242	-5.254	19.082	1.00	7.97
ATOM	939	CG	GLU	222	-3.344	-6.131	20.308	1.00	9.39
ATOM	940	CD	GLU	222	-4.417	-7.198	20.200	1.00	10.45
ATOM	941	OE1	GLU	222	-4.780	-7.583	19.067	1.00	8.96
ATOM	942	OE2	GLU	222	-4.877	-7.675	21.258	1.00	9.57
ATOM	943	C	GLU	222	-4.610	-3.342	20.001	1.00	9.11
ATOM	944	O	GLU	222	-5.577	-3.433	20.754	1.00	9.41
ATOM	945	N	TYR	223	-3.686	-2.400	20.125	1.00	8.02
ATOM	946	CA	TYR	223	-3.717	-1.412	21.193	1.00	9.53
ATOM	947	CB	TYR	223	-2.532	-0.466	21.013	1.00	8.20
ATOM	948	CG	TYR	223	-2.509	0.722	21.944	1.00	11.39
ATOM	949	CD1	TYR	223	-2.527	0.550	23.326	1.00	10.93
ATOM	950	CE1	TYR	223	-2.434	1.647	24.189	1.00	11.93
ATOM	951	CD2	TYR	223	-2.408	2.021	21.441	1.00	11.57
ATOM	952	CE2	TYR	223	-2.318	3.123	22.294	1.00	10.97
ATOM	953	CZ	TYR	223	-2.327	2.924	23.664	1.00	11.57
ATOM	954	OH	TYR	223	-2.199	3.997	24.515	1.00	9.92
ATOM	955	C	TYR	223	-5.033	-0.628	21.222	1.00	8.48
ATOM	956	O	TYR	223	-5.704	-0.549	22.258	1.00	7.47
ATOM	957	N	PHE	224	-5.415	-0.062	20.083	1.00	8.20
ATOM	958	CA	PHE	224	-6.644	0.711	20.025	1.00	9.95
ATOM	959	CB	PHE	224	-6.652	1.585	18.764	1.00	8.57
ATOM	960	CG	PHE	224	-5.679	2.730	18.835	1.00	8.93
ATOM	961	CD1	PHE	224	-4.481	2.698	18.130	1.00	7.84
ATOM	962	CD2	PHE	224	-5.939	3.816	19.668	1.00	8.53
ATOM	963	CE1	PHE	224	-3.548	3.733	18.257	1.00	8.93
ATOM	964	CE2	PHE	224	-5.020	4.850	19.804	1.00	9.21

ATOM	965	CZ	PHE	224	-3.819	4.809	19.096	1.00	8.88
ATOM	966	C	PHE	224	-7.940	-0.098	20.136	1.00	11.22
ATOM	967	O	PHE	224	-8.924	0.412	20.671	1.00	12.10
ATOM	968	N	GLN	225	-7.964	-1.338	19.648	1.00	12.77
ATOM	969	CA	GLN	225	-9.195	-2.131	19.772	1.00	12.94
ATOM	970	CB	GLN	225	-9.161	-3.372	18.870	1.00	16.76
ATOM	971	CG	GLN	225	-10.435	-4.260	18.911	1.00	19.91
ATOM	972	CD	GLN	225	-11.744	-3.516	18.577	1.00	25.45
ATOM	973	OE1	GLN	225	-12.366	-2.882	19.449	1.00	27.22
ATOM	974	NE2	GLN	225	-12.162	-3.591	17.311	1.00	25.02
ATOM	975	C	GLN	225	-9.376	-2.545	21.232	1.00	11.68
ATOM	976	O	GLN	225	-10.489	-2.769	21.689	1.00	11.15
ATOM	977	N	ALA	226	-8.281	-2.642	21.974	1.00	13.05
ATOM	978	CA	ALA	226	-8.382	-3.019	23.377	1.00	12.70
ATOM	979	CB	ALA	226	-7.070	-3.655	23.852	1.00	11.29
ATOM	980	C	ALA	226	-8.747	-1.833	24.274	1.00	12.83
ATOM	981	O	ALA	226	-9.445	-2.008	25.279	1.00	12.14
ATOM	982	N	THR	227	-8.292	-0.631	23.918	1.00	11.74
ATOM	983	CA	THR	227	-8.573	0.545	24.731	1.00	11.76
ATOM	984	CB	THR	227	-7.377	1.552	24.726	1.00	12.18
ATOM	985	OG1	THR	227	-7.070	1.952	23.380	1.00	10.40
ATOM	986	CG2	THR	227	-6.141	0.913	25.374	1.00	11.11
ATOM	987	C	THR	227	-9.852	1.301	24.358	1.00	12.48
ATOM	988	O	THR	227	-10.331	2.137	25.132	1.00	11.05
ATOM	989	N	TYR	228	-10.409	1.009	23.187	1.00	12.51
ATOM	990	CA	TYR	228	-11.639	1.674	22.758	1.00	14.63
ATOM	991	CB	TYR	228	-12.068	1.132	21.390	1.00	17.13
ATOM	992	CG	TYR	228	-13.414	1.623	20.916	1.00	19.18
ATOM	993	CD1	TYR	228	-13.653	2.981	20.712	1.00	20.44
ATOM	994	CE1	TYR	228	-14.897	3.437	20.270	1.00	20.05
ATOM	995	CD2	TYR	228	-14.453	0.724	20.667	1.00	20.84
ATOM	996	CE2	TYR	228	-15.698	1.164	20.224	1.00	22.27
ATOM	997	CZ	TYR	228	-15.912	2.520	20.029	1.00	21.39
ATOM	998	OH	TYR	228	-17.140	2.956	19.598	1.00	22.61
ATOM	999	C	TYR	228	-12.773	1.497	23.789	1.00	13.80
ATOM	1000	O	TYR	228	-13.463	2.454	24.134	1.00	11.95
ATOM	1001	N	PRO	229	-12.975	0.268	24.295	1.00	14.35
ATOM	1002	CD	PRO	229	-12.320	-1.002	23.930	1.00	15.39
ATOM	1003	CA	PRO	229	-14.040	0.043	25.282	1.00	14.36
ATOM	1004	CB	PRO	229	-13.921	-1.449	25.594	1.00	16.35
ATOM	1005	CG	PRO	229	-13.376	-2.023	24.305	1.00	17.63
ATOM	1006	C	PRO	229	-13.856	0.891	26.540	1.00	13.84
ATOM	1007	O	PRO	229	-14.832	1.317	27.160	1.00	13.57
ATOM	1008	N	LEU	230	-12.600	1.123	26.918	1.00	12.78
ATOM	1009	CA	LEU	230	-12.296	1.916	28.102	1.00	14.44
ATOM	1010	CB	LEU	230	-10.808	1.819	28.443	1.00	15.85
ATOM	1011	CG	LEU	230	-10.364	1.179	29.755	1.00	20.81
ATOM	1012	CD1	LEU	230	-8.910	1.559	29.981	1.00	22.31
ATOM	1013	CD2	LEU	230	-11.215	1.657	30.926	1.00	20.68
ATOM	1014	C	LEU	230	-12.662	3.378	27.872	1.00	13.88
ATOM	1015	O	LEU	230	-13.193	4.045	28.760	1.00	12.99
ATOM	1016	N	LEU	231	-12.372	3.872	26.676	1.00	15.59
ATOM	1017	CA	LEU	231	-12.673	5.257	26.340	1.00	17.53
ATOM	1018	CB	LEU	231	-12.101	5.610	24.962	1.00	14.45
ATOM	1019	CG	LEU	231	-12.246	7.078	24.559	1.00	15.09
ATOM	1020	CD1	LEU	231	-11.662	7.970	25.648	1.00	11.11
ATOM	1021	CD2	LEU	231	-11.547	7.319	23.221	1.00	13.00
ATOM	1022	C	LEU	231	-14.181	5.480	26.352	1.00	18.31
ATOM	1023	O	LEU	231	-14.660	6.535	26.772	1.00	19.08
ATOM	1024	N	LYS	232	-14.929	4.481	25.902	1.00	19.55
ATOM	1025	CA	LYS	232	-16.384	4.593	25.875	1.00	21.84
ATOM	1026	CB	LYS	232	-16.997	3.521	24.971	1.00	23.94
ATOM	1027	CG	LYS	232	-17.286	3.978	23.552	1.00	26.52
ATOM	1028	CD	LYS	232	-18.411	3.156	22.938	1.00	30.98
ATOM	1029	CE	LYS	232	-18.077	1.663	22.910	1.00	33.24
ATOM	1030	NZ	LYS	232	-19.208	0.837	22.379	1.00	34.79
ATOM	1031	C	LYS	232	-17.018	4.480	27.256	1.00	21.69

ATOM	1032	O	LYS	232	-18.077	5.060	27.502	1.00	22.17
ATOM	1033	N	ALA	233	-16.365	3.747	28.155	1.00	19.96
ATOM	1034	CA	ALA	233	-16.899	3.525	29.497	1.00	20.23
ATOM	1035	CB	ALA	233	-16.583	2.095	29.942	1.00	19.82
ATOM	1036	C	ALA	233	-16.459	4.495	30.584	1.00	19.94
ATOM	1037	O	ALA	233	-17.073	4.545	31.656	1.00	22.42
ATOM	1038	N	ASP	234	-15.407	5.262	30.330	1.00	17.64
ATOM	1039	CA	ASP	234	-14.914	6.199	31.330	1.00	15.26
ATOM	1040	CB	ASP	234	-13.516	5.761	31.773	1.00	16.13
ATOM	1041	CG	ASP	234	-12.986	6.572	32.929	1.00	13.28
ATOM	1042	OD1	ASP	234	-13.635	7.562	33.333	1.00	13.38
ATOM	1043	OD2	ASP	234	-11.901	6.218	33.434	1.00	16.02
ATOM	1044	C	ASP	234	-14.876	7.621	30.756	1.00	15.97
ATOM	1045	O	ASP	234	-13.958	7.974	30.018	1.00	14.93
ATOM	1046	N	PRO	235	-15.887	8.447	31.086	1.00	15.09
ATOM	1047	CD	PRO	235	-17.040	8.086	31.933	1.00	14.73
ATOM	1048	CA	PRO	235	-16.004	9.835	30.619	1.00	14.22
ATOM	1049	CB	PRO	235	-17.399	10.244	31.091	1.00	13.06
ATOM	1050	CG	PRO	235	-17.568	9.445	32.353	1.00	14.04
ATOM	1051	C	PRO	235	-14.911	10.771	31.127	1.00	13.90
ATOM	1052	O	PRO	235	-14.796	11.909	30.658	1.00	15.31
ATOM	1053	N	SER	236	-14.117	10.304	32.088	1.00	12.39
ATOM	1054	CA	SER	236	-13.024	11.126	32.605	1.00	9.37
ATOM	1055	CB	SER	236	-12.634	10.685	34.026	1.00	7.86
ATOM	1056	OG	SER	236	-12.025	9.409	34.035	1.00	11.01
ATOM	1057	C	SER	236	-11.841	10.978	31.638	1.00	9.06
ATOM	1058	O	SER	236	-10.818	11.651	31.769	1.00	8.77
ATOM	1059	N	LEU	237	-11.994	10.082	30.668	1.00	8.71
ATOM	1060	CA	LEU	237	-10.979	9.863	29.635	1.00	10.57
ATOM	1061	CB	LEU	237	-10.792	8.369	29.354	1.00	8.21
ATOM	1062	CG	LEU	237	-10.017	7.485	30.334	1.00	10.83
ATOM	1063	CD1	LEU	237	-10.028	6.043	29.827	1.00	10.32
ATOM	1064	CD2	LEU	237	-8.590	8.008	30.473	1.00	10.36
ATOM	1065	C	LEU	237	-11.510	10.515	28.366	1.00	10.55
ATOM	1066	O	LEU	237	-12.688	10.352	28.034	1.00	10.74
ATOM	1067	N	TRP	238	-10.670	11.254	27.646	1.00	12.42
ATOM	1068	CA	TRP	238	-11.150	11.865	26.414	1.00	10.23
ATOM	1069	CB	TRP	238	-11.233	13.398	26.568	1.00	11.21
ATOM	1070	CG	TRP	238	-9.948	14.177	26.472	1.00	12.18
ATOM	1071	CD2	TRP	238	-9.805	15.522	25.992	1.00	12.22
ATOM	1072	CE2	TRP	238	-8.443	15.874	26.126	1.00	13.26
ATOM	1073	CE3	TRP	238	-10.698	16.464	25.463	1.00	12.35
ATOM	1074	CD1	TRP	238	-8.702	13.778	26.868	1.00	12.73
ATOM	1075	NE1	TRP	238	-7.791	14.793	26.660	1.00	14.85
ATOM	1076	CZ2	TRP	238	-7.952	17.130	25.748	1.00	13.99
ATOM	1077	CZ3	TRP	238	-10.209	17.713	25.085	1.00	13.96
ATOM	1078	CH2	TRP	238	-8.847	18.032	25.230	1.00	14.06
ATOM	1079	C	TRP	238	-10.326	11.448	25.194	1.00	10.61
ATOM	1080	O	TRP	238	-10.580	11.894	24.074	1.00	9.29
ATOM	1081	N	CYS	239	-9.360	10.557	25.408	1.00	9.82
ATOM	1082	CA	CYS	239	-8.534	10.071	24.309	1.00	11.22
ATOM	1083	C	CYS	239	-7.606	8.923	24.673	1.00	10.30
ATOM	1084	O	CYS	239	-7.358	8.654	25.847	1.00	9.57
ATOM	1085	CB	CYS	239	-7.727	11.239	23.728	1.00	14.41
ATOM	1086	SG	CYS	239	-5.902	11.260	23.866	1.00	14.48
ATOM	1087	N	VAL	240	-7.135	8.221	23.648	1.00	9.37
ATOM	1088	CA	VAL	240	-6.183	7.134	23.817	1.00	9.33
ATOM	1089	CB	VAL	240	-6.798	5.750	23.511	1.00	8.77
ATOM	1090	CG1	VAL	240	-5.716	4.654	23.633	1.00	6.55
ATOM	1091	CG2	VAL	240	-7.938	5.462	24.495	1.00	7.87
ATOM	1092	C	VAL	240	-5.083	7.456	22.814	1.00	9.68
ATOM	1093	O	VAL	240	-5.323	7.506	21.601	1.00	10.65
ATOM	1094	N	SER	241	-3.879	7.692	23.325	1.00	10.79
ATOM	1095	CA	SER	241	-2.746	8.049	22.480	1.00	9.68
ATOM	1096	CB	SER	241	-2.143	9.377	22.960	1.00	9.93
ATOM	1097	OG	SER	241	-0.985	9.716	22.214	1.00	9.51
ATOM	1098	C	SER	241	-1.668	6.970	22.463	1.00	9.59

ATOM	1099	O	SER	241	-1.459	6.261	23.449	1.00	8.78
ATOM	1100	N	ALA	242	-0.996	6.845	21.326	1.00	9.62
ATOM	1101	CA	ALA	242	0.070	5.866	21.156	1.00	8.54
ATOM	1102	CB	ALA	242	0.172	5.482	19.686	1.00	7.74
ATOM	1103	C	ALA	242	1.402	6.447	21.612	1.00	9.09
ATOM	1104	O	ALA	242	2.399	5.732	21.732	1.00	11.19
ATOM	1105	N	TRP	243	1.402	7.741	21.903	1.00	8.70
ATOM	1106	CA	TRP	243	2.625	8.460	22.243	1.00	9.33
ATOM	1107	CB	TRP	243	2.563	9.820	21.530	1.00	8.85
ATOM	1108	CG	TRP	243	3.866	10.562	21.410	1.00	10.62
ATOM	1109	CD2	TRP	243	4.832	10.424	20.361	1.00	12.62
ATOM	1110	CE2	TRP	243	5.887	11.323	20.640	1.00	13.42
ATOM	1111	CE3	TRP	243	4.909	9.628	19.210	1.00	10.66
ATOM	1112	CD1	TRP	243	4.359	11.510	22.263	1.00	13.59
ATOM	1113	NE1	TRP	243	5.575	11.976	21.805	1.00	13.28
ATOM	1114	CZ2	TRP	243	7.004	11.448	19.809	1.00	14.45
ATOM	1115	CZ3	TRP	243	6.024	9.753	18.379	1.00	12.64
ATOM	1116	CH2	TRP	243	7.056	10.658	18.687	1.00	12.62
ATOM	1117	C	TRP	243	3.036	8.670	23.702	1.00	10.76
ATOM	1118	O	TRP	243	2.242	9.112	24.541	1.00	11.13
ATOM	1119	N	ASN	244	4.293	8.337	23.996	1.00	8.80
ATOM	1120	CA	ASN	244	4.856	8.568	25.327	1.00	9.77
ATOM	1121	CB	ASN	244	5.634	7.346	25.843	1.00	8.88
ATOM	1122	CG	ASN	244	6.369	7.638	27.157	1.00	11.44
ATOM	1123	OD1	ASN	244	6.315	8.760	27.666	1.00	11.69
ATOM	1124	ND2	ASN	244	7.055	6.638	27.704	1.00	9.32
ATOM	1125	C	ASN	244	5.821	9.732	25.096	1.00	9.64
ATOM	1126	O	ASN	244	6.861	9.561	24.454	1.00	9.06
ATOM	1127	N	ASP	245	5.474	10.916	25.596	1.00	9.77
ATOM	1128	CA	ASP	245	6.305	12.107	25.406	1.00	11.66
ATOM	1129	CB	ASP	245	5.639	13.311	26.077	1.00	11.31
ATOM	1130	CG	ASP	245	4.471	13.843	25.269	1.00	14.43
ATOM	1131	OD1	ASP	245	4.715	14.521	24.247	1.00	12.83
ATOM	1132	OD2	ASP	245	3.305	13.573	25.641	1.00	15.01
ATOM	1133	C	ASP	245	7.757	11.979	25.872	1.00	12.16
ATOM	1134	O	ASP	245	8.637	12.681	25.369	1.00	11.24
ATOM	1135	N	ASN	246	8.001	11.091	26.832	1.00	13.24
ATOM	1136	CA	ASN	246	9.345	10.857	27.347	1.00	13.37
ATOM	1137	CB	ASN	246	9.365	11.037	28.867	1.00	14.88
ATOM	1138	CG	ASN	246	9.067	12.461	29.288	1.00	15.35
ATOM	1139	OD1	ASN	246	9.798	13.390	28.934	1.00	17.50
ATOM	1140	ND2	ASN	246	7.987	12.645	30.041	1.00	13.52
ATOM	1141	C	ASN	246	9.783	9.434	26.994	1.00	14.92
ATOM	1142	O	ASN	246	10.619	8.842	27.676	1.00	15.41
ATOM	1143	N	GLY	247	9.221	8.900	25.912	1.00	14.67
ATOM	1144	CA	GLY	247	9.530	7.542	25.504	1.00	14.92
ATOM	1145	C	GLY	247	10.843	7.261	24.789	1.00	15.80
ATOM	1146	O	GLY	247	10.857	6.518	23.804	1.00	15.10
ATOM	1147	N	LYS	248	11.941	7.843	25.263	1.00	15.12
ATOM	1148	CA	LYS	248	13.243	7.598	24.654	1.00	16.23
ATOM	1149	CB	LYS	248	14.262	8.633	25.135	1.00	19.28
ATOM	1150	CG	LYS	248	13.886	10.079	24.822	1.00	21.61
ATOM	1151	CD	LYS	248	14.985	11.013	25.304	1.00	25.34
ATOM	1152	CE	LYS	248	14.644	12.472	25.079	1.00	27.00
ATOM	1153	NZ	LYS	248	15.740	13.345	25.617	1.00	27.20
ATOM	1154	C	LYS	248	13.675	6.188	25.070	1.00	16.55
ATOM	1155	O	LYS	248	13.198	5.670	26.080	1.00	15.38
ATOM	1156	N	GLU	249	14.575	5.572	24.307	1.00	16.15
ATOM	1157	CA	GLU	249	15.004	4.204	24.598	1.00	15.56
ATOM	1158	CB	GLU	249	16.070	3.744	23.592	1.00	18.49
ATOM	1159	CG	GLU	249	16.478	2.264	23.751	1.00	23.13
ATOM	1160	CD	GLU	249	17.586	1.835	22.786	1.00	26.95
ATOM	1161	OE1	GLU	249	17.324	1.721	21.568	1.00	30.01
ATOM	1162	OE2	GLU	249	18.729	1.616	23.244	1.00	28.21
ATOM	1163	C	GLU	249	15.500	3.922	26.015	1.00	13.54
ATOM	1164	O	GLU	249	15.081	2.945	26.623	1.00	13.46
ATOM	1165	N	GLN	250	16.389	4.754	26.546	1.00	12.48

ATOM	1166	CA	GLN	250	16.909	4.513	27.888	1.00	13.33
ATOM	1167	CB	GLN	250	18.284	5.172	28.064	1.00	15.06
ATOM	1168	CG	GLN	250	19.386	4.613	27.162	1.00	17.76
ATOM	1169	CD	GLN	250	19.550	3.104	27.284	1.00	18.56
ATOM	1170	OE1	GLN	250	19.724	2.566	28.383	1.00	20.45
ATOM	1171	NE2	GLN	250	19.501	2.414	26.150	1.00	20.59
ATOM	1172	C	GLN	250	15.974	4.992	28.998	1.00	12.47
ATOM	1173	O	GLN	250	16.313	4.896	30.178	1.00	11.69
ATOM	1174	N	MET	251	14.799	5.493	28.624	1.00	11.56
ATOM	1175	CA	MET	251	13.846	5.980	29.608	1.00	11.87
ATOM	1176	CB	MET	251	13.525	7.448	29.337	1.00	12.21
ATOM	1177	CG	MET	251	14.707	8.369	29.657	1.00	14.77
ATOM	1178	SD	MET	251	14.378	10.087	29.329	1.00	21.33
ATOM	1179	CE	MET	251	13.550	10.533	30.819	1.00	17.14
ATOM	1180	C	MET	251	12.559	5.173	29.713	1.00	12.06
ATOM	1181	O	MET	251	11.617	5.592	30.387	1.00	10.10
ATOM	1182	N	VAL	252	12.516	4.027	29.038	1.00	11.58
ATOM	1183	CA	VAL	252	11.350	3.153	29.087	1.00	10.03
ATOM	1184	CB	VAL	252	10.585	3.107	27.730	1.00	7.93
ATOM	1185	CG1	VAL	252	10.194	4.517	27.300	1.00	9.58
ATOM	1186	CG2	VAL	252	11.444	2.445	26.656	1.00	8.14
ATOM	1187	C	VAL	252	11.818	1.742	29.446	1.00	12.90
ATOM	1188	O	VAL	252	12.951	1.353	29.120	1.00	11.82
ATOM	1189	N	ASP	253	10.944	0.995	30.121	1.00	11.34
ATOM	1190	CA	ASP	253	11.213	-0.381	30.553	1.00	12.33
ATOM	1191	CB	ASP	253	10.410	-0.689	31.825	1.00	12.26
ATOM	1192	CG	ASP	253	10.788	-2.020	32.457	1.00	12.19
ATOM	1193	OD1	ASP	253	11.378	-2.883	31.769	1.00	12.10
ATOM	1194	OD2	ASP	253	10.480	-2.209	33.654	1.00	11.59
ATOM	1195	C	ASP	253	10.802	-1.352	29.446	1.00	13.89
ATOM	1196	O	ASP	253	9.613	-1.651	29.273	1.00	14.95
ATOM	1197	N	SER	254	11.785	-1.859	28.706	1.00	13.84
ATOM	1198	CA	SER	254	11.498	-2.773	27.607	1.00	15.02
ATOM	1199	CB	SER	254	12.767	-3.022	26.786	1.00	16.06
ATOM	1200	OG	SER	254	13.804	-3.529	27.608	1.00	20.55
ATOM	1201	C	SER	254	10.895	-4.104	28.041	1.00	14.12
ATOM	1202	O	SER	254	10.424	-4.867	27.197	1.00	13.00
ATOM	1203	N	SER	255	10.909	-4.387	29.345	1.00	12.60
ATOM	1204	CA	SER	255	10.347	-5.637	29.853	1.00	11.71
ATOM	1205	CB	SER	255	11.125	-6.135	31.079	1.00	10.16
ATOM	1206	OG	SER	255	10.791	-5.405	32.251	1.00	10.89
ATOM	1207	C	SER	255	8.876	-5.468	30.217	1.00	12.25
ATOM	1208	O	SER	255	8.227	-6.415	30.671	1.00	12.47
ATOM	1209	N	LYS	256	8.354	-4.256	30.026	1.00	10.86
ATOM	1210	CA	LYS	256	6.940	-3.980	30.296	1.00	9.20
ATOM	1211	CB	LYS	256	6.777	-3.093	31.535	1.00	9.79
ATOM	1212	CG	LYS	256	7.075	-3.792	32.872	1.00	11.34
ATOM	1213	CD	LYS	256	6.182	-5.022	33.107	1.00	14.09
ATOM	1214	CE	LYS	256	4.790	-4.662	33.642	1.00	13.97
ATOM	1215	NZ	LYS	256	4.135	-3.625	32.811	1.00	22.97
ATOM	1216	C	LYS	256	6.311	-3.282	29.092	1.00	8.79
ATOM	1217	O	LYS	256	5.760	-2.195	29.220	1.00	6.68
ATOM	1218	N	PRO	257	6.373	-3.900	27.902	1.00	7.71
ATOM	1219	CD	PRO	257	6.884	-5.229	27.506	1.00	7.22
ATOM	1220	CA	PRO	257	5.765	-3.204	26.765	1.00	7.07
ATOM	1221	CB	PRO	257	6.238	-4.024	25.573	1.00	6.88
ATOM	1222	CG	PRO	257	6.237	-5.440	26.140	1.00	7.20
ATOM	1223	C	PRO	257	4.239	-3.116	26.864	1.00	8.43
ATOM	1224	O	PRO	257	3.597	-2.370	26.109	1.00	8.84
ATOM	1225	N	GLU	258	3.661	-3.855	27.810	1.00	7.72
ATOM	1226	CA	GLU	258	2.211	-3.864	27.989	1.00	7.04
ATOM	1227	CB	GLU	258	1.736	-5.247	28.487	1.00	10.40
ATOM	1228	CG	GLU	258	1.968	-5.520	29.987	1.00	11.44
ATOM	1229	CD	GLU	258	3.338	-6.132	30.302	1.00	13.80
ATOM	1230	OE1	GLU	258	4.290	-5.941	29.518	1.00	13.19
ATOM	1231	OE2	GLU	258	3.467	-6.794	31.350	1.00	13.15
ATOM	1232	C	GLU	258	1.731	-2.794	28.968	1.00	9.11

ATOM	1233	O	GLU	258	0.544	-2.481	29.017	1.00	9.03
ATOM	1234	N	LEU	259	2.651	-2.230	29.744	1.00	8.14
ATOM	1235	CA	LEU	259	2.290	-1.224	30.746	1.00	7.54
ATOM	1236	CB	LEU	259	3.505	-0.882	31.606	1.00	6.24
ATOM	1237	CG	LEU	259	3.229	0.083	32.762	1.00	8.45
ATOM	1238	CD1	LEU	259	2.112	-0.462	33.637	1.00	7.48
ATOM	1239	CD2	LEU	259	4.501	0.280	33.561	1.00	9.63
ATOM	1240	C	LEU	259	1.696	0.061	30.174	1.00	7.01
ATOM	1241	O	LEU	259	2.286	0.692	29.300	1.00	8.51
ATOM	1242	N	LEU	260	0.524	0.445	30.673	1.00	7.32
ATOM	1243	CA	LEU	260	-0.139	1.666	30.218	1.00	9.34
ATOM	1244	CB	LEU	260	-1.503	1.351	29.592	1.00	9.36
ATOM	1245	CG	LEU	260	-1.498	0.340	28.453	1.00	7.44
ATOM	1246	CD1	LEU	260	-2.925	0.134	27.953	1.00	8.83
ATOM	1247	CD2	LEU	260	-0.593	0.839	27.330	1.00	9.07
ATOM	1248	C	LEU	260	-0.340	2.634	31.379	1.00	9.85
ATOM	1249	O	LEU	260	-0.262	2.237	32.547	1.00	10.96
ATOM	1250	N	TYR	261	-0.610	3.897	31.041	1.00	9.78
ATOM	1251	CA	TYR	261	-0.815	4.958	32.026	1.00	9.25
ATOM	1252	CB	TYR	261	0.445	5.821	32.170	1.00	8.23
ATOM	1253	CG	TYR	261	1.722	5.127	32.590	1.00	9.29
ATOM	1254	CD1	TYR	261	2.520	4.455	31.667	1.00	10.68
ATOM	1255	CE1	TYR	261	3.737	3.881	32.055	1.00	8.99
ATOM	1256	CD2	TYR	261	2.164	5.203	33.909	1.00	10.08
ATOM	1257	CE2	TYR	261	3.359	4.639	34.302	1.00	9.05
ATOM	1258	CZ	TYR	261	4.143	3.982	33.378	1.00	9.04
ATOM	1259	OH	TYR	261	5.326	3.417	33.794	1.00	8.78
ATOM	1260	C	TYR	261	-1.925	5.927	31.623	1.00	9.98
ATOM	1261	O	TYR	261	-2.434	5.894	30.499	1.00	10.51
ATOM	1262	N	ARG	262	-2.269	6.805	32.561	1.00	10.88
ATOM	1263	CA	ARG	262	-3.227	7.876	32.328	1.00	10.37
ATOM	1264	CB	ARG	262	-4.226	8.015	33.496	1.00	11.25
ATOM	1265	CG	ARG	262	-5.339	6.954	33.553	1.00	10.96
ATOM	1266	CD	ARG	262	-6.291	7.201	34.738	1.00	11.63
ATOM	1267	NE	ARG	262	-7.169	8.358	34.539	1.00	11.87
ATOM	1268	CZ	ARG	262	-8.442	8.277	34.151	1.00	11.29
ATOM	1269	NH1	ARG	262	-8.999	7.093	33.919	1.00	9.97
ATOM	1270	NH2	ARG	262	-9.164	9.380	33.992	1.00	13.25
ATOM	1271	C	ARG	262	-2.328	9.122	32.285	1.00	11.39
ATOM	1272	O	ARG	262	-1.294	9.160	32.970	1.00	10.60
ATOM	1273	N	THR	263	-2.689	10.112	31.467	1.00	10.18
ATOM	1274	CA	THR	263	-1.936	11.375	31.392	1.00	9.51
ATOM	1275	CB	THR	263	-0.879	11.394	30.256	1.00	8.82
ATOM	1276	OG1	THR	263	-0.227	12.675	30.249	1.00	8.34
ATOM	1277	CG2	THR	263	-1.529	11.179	28.902	1.00	5.53
ATOM	1278	C	THR	263	-2.857	12.575	31.161	1.00	11.03
ATOM	1279	O	THR	263	-3.810	12.499	30.379	1.00	11.68
ATOM	1280	N	ASP	264	-2.562	13.679	31.847	1.00	9.41
ATOM	1281	CA	ASP	264	-3.334	14.916	31.717	1.00	10.91
ATOM	1282	CB	ASP	264	-3.140	15.797	32.960	1.00	8.53
ATOM	1283	CG	ASP	264	-3.821	15.232	34.190	1.00	9.31
ATOM	1284	OD1	ASP	264	-3.210	15.270	35.287	1.00	10.37
ATOM	1285	OD2	ASP	264	-4.976	14.766	34.065	1.00	6.68
ATOM	1286	C	ASP	264	-2.857	15.675	30.484	1.00	10.78
ATOM	1287	O	ASP	264	-3.566	16.536	29.951	1.00	11.64
ATOM	1288	N	PHE	265	-1.651	15.339	30.031	1.00	10.62
ATOM	1289	CA	PHE	265	-1.035	15.976	28.872	1.00	9.79
ATOM	1290	CB	PHE	265	0.496	15.977	29.035	1.00	9.23
ATOM	1291	CG	PHE	265	1.219	16.899	28.076	1.00	10.18
ATOM	1292	CD1	PHE	265	1.590	18.179	28.467	1.00	9.63
ATOM	1293	CD2	PHE	265	1.517	16.485	26.774	1.00	9.73
ATOM	1294	CE1	PHE	265	2.246	19.036	27.582	1.00	8.95
ATOM	1295	CE2	PHE	265	2.171	17.334	25.883	1.00	6.84
ATOM	1296	CZ	PHE	265	2.536	18.607	26.283	1.00	8.37
ATOM	1297	C	PHE	265	-1.416	15.254	27.571	1.00	9.45
ATOM	1298	O	PHE	265	-0.991	14.113	27.325	1.00	7.59
ATOM	1299	N	PHE	266	-2.221	15.929	26.748	1.00	8.26

ATOM	1300	CA	PHE	266	-2.666	15.398	25.461	1.00	8.23
ATOM	1301	CB	PHE	266	-3.646	16.380	24.805	1.00	7.58
ATOM	1302	CG	PHE	266	-4.065	15.978	23.419	1.00	9.94
ATOM	1303	CD1	PHE	266	-4.785	14.803	23.213	1.00	10.74
ATOM	1304	CD2	PHE	266	-3.717	16.752	22.320	1.00	8.83
ATOM	1305	CE1	PHE	266	-5.152	14.403	21.930	1.00	11.66
ATOM	1306	CE2	PHE	266	-4.077	16.360	21.030	1.00	7.16
ATOM	1307	CZ	PHE	266	-4.796	15.187	20.834	1.00	9.59
ATOM	1308	C	PHE	266	-1.446	15.201	24.553	1.00	8.37
ATOM	1309	O	PHE	266	-0.783	16.179	24.170	1.00	9.54
ATOM	1310	N	PRO	267	-1.135	13.942	24.184	1.00	7.74
ATOM	1311	CD	PRO	267	-1.627	12.700	24.804	1.00	6.83
ATOM	1312	CA	PRO	267	0.024	13.648	23.321	1.00	7.06
ATOM	1313	CB	PRO	267	0.412	12.222	23.727	1.00	5.62
ATOM	1314	CG	PRO	267	-0.345	11.973	25.040	1.00	7.56
ATOM	1315	C	PRO	267	-0.200	13.723	21.811	1.00	6.68
ATOM	1316	O	PRO	267	0.727	14.020	21.062	1.00	6.65
ATOM	1317	N	GLY	268	-1.420	13.438	21.367	1.00	7.45
ATOM	1318	CA	GLY	268	-1.693	13.450	19.941	1.00	9.64
ATOM	1319	C	GLY	268	-0.847	12.339	19.345	1.00	10.08
ATOM	1320	O	GLY	268	-0.754	11.249	19.923	1.00	9.01
ATOM	1321	N	LEU	269	-0.234	12.614	18.197	1.00	9.24
ATOM	1322	CA	LEU	269	0.639	11.661	17.512	1.00	9.76
ATOM	1323	CB	LEU	269	2.048	11.757	18.114	1.00	9.55
ATOM	1324	CG	LEU	269	2.592	13.184	17.932	1.00	9.11
ATOM	1325	CD1	LEU	269	3.882	13.388	18.721	1.00	9.82
ATOM	1326	CD2	LEU	269	2.799	13.437	16.443	1.00	6.64
ATOM	1327	C	LEU	269	0.134	10.217	17.536	1.00	9.61
ATOM	1328	O	LEU	269	0.757	9.335	18.118	1.00	10.92
ATOM	1329	N	GLY	270	-0.983	9.984	16.851	1.00	9.28
ATOM	1330	CA	GLY	270	-1.586	8.666	16.823	1.00	9.10
ATOM	1331	C	GLY	270	-2.551	8.631	17.992	1.00	11.07
ATOM	1332	O	GLY	270	-2.214	8.128	19.064	1.00	10.01
ATOM	1333	N	TRP	271	-3.750	9.173	17.800	1.00	11.13
ATOM	1334	CA	TRP	271	-4.725	9.208	18.888	1.00	11.80
ATOM	1335	CB	TRP	271	-4.672	10.549	19.620	1.00	10.94
ATOM	1336	CG	TRP	271	-4.959	11.736	18.749	1.00	11.28
ATOM	1337	CD2	TRP	271	-6.113	12.583	18.801	1.00	9.48
ATOM	1338	CE2	TRP	271	-5.931	13.597	17.832	1.00	11.44
ATOM	1339	CE3	TRP	271	-7.283	12.588	19.574	1.00	11.08
ATOM	1340	CD1	TRP	271	-4.149	12.252	17.774	1.00	9.73
ATOM	1341	NE1	TRP	271	-4.726	13.369	17.222	1.00	9.69
ATOM	1342	CZ2	TRP	271	-6.876	14.609	17.614	1.00	9.00
ATOM	1343	CZ3	TRP	271	-8.223	13.595	19.360	1.00	10.91
ATOM	1344	CH2	TRP	271	-8.009	14.594	18.383	1.00	11.46
ATOM	1345	C	TRP	271	-6.157	8.941	18.476	1.00	11.82
ATOM	1346	O	TRP	271	-6.602	9.346	17.399	1.00	12.33
ATOM	1347	N	LEU	272	-6.869	8.266	19.371	1.00	11.04
ATOM	1348	CA	LEU	272	-8.264	7.901	19.186	1.00	11.53
ATOM	1349	CB	LEU	272	-8.479	6.480	19.720	1.00	10.97
ATOM	1350	CG	LEU	272	-9.904	5.961	19.933	1.00	11.77
ATOM	1351	CD1	LEU	272	-10.522	5.554	18.598	1.00	9.05
ATOM	1352	CD2	LEU	272	-9.862	4.771	20.883	1.00	9.57
ATOM	1353	C	LEU	272	-9.215	8.858	19.916	1.00	10.97
ATOM	1354	O	LEU	272	-8.989	9.218	21.072	1.00	9.88
ATOM	1355	N	LEU	273	-10.276	9.274	19.237	1.00	11.08
ATOM	1356	CA	LEU	273	-11.267	10.131	19.869	1.00	9.85
ATOM	1357	CB	LEU	273	-11.137	11.587	19.409	1.00	8.45
ATOM	1358	CG	LEU	273	-11.638	12.045	18.037	1.00	9.35
ATOM	1359	CD1	LEU	273	-11.658	13.573	18.030	1.00	9.10
ATOM	1360	CD2	LEU	273	-10.753	11.526	16.914	1.00	5.46
ATOM	1361	C	LEU	273	-12.643	9.590	19.511	1.00	10.70
ATOM	1362	O	LEU	273	-12.799	8.869	18.522	1.00	8.50
ATOM	1363	N	LEU	274	-13.633	9.908	20.335	1.00	10.98
ATOM	1364	CA	LEU	274	-14.994	9.466	20.071	1.00	10.84
ATOM	1365	CB	LEU	274	-15.724	9.163	21.374	1.00	7.85
ATOM	1366	CG	LEU	274	-15.141	8.028	22.210	1.00	6.58

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ATOM   1367  CD1 LEU   274     -15.975   7.880  23.481  1.00  6.55
ATOM   1368  CD2 LEU   274     -15.135   6.736  21.420  1.00  5.23
ATOM   1369  C   LEU   274     -15.744  10.561  19.338  1.00 10.09
ATOM   1370  O   LEU   274     -15.401  11.735  19.437  1.00 10.18
ATOM   1371  N   ALA   275     -16.767  10.165  18.597  1.00 13.02
ATOM   1372  CA  ALA   275     -17.579  11.119  17.865  1.00 11.86
ATOM   1373  CB  ALA   275     -18.709  10.400  17.138  1.00 11.74
ATOM   1374  C   ALA   275     -18.138  12.086  18.895  1.00 12.51
ATOM   1375  O   ALA   275     -18.368  13.248  18.588  1.00 11.85
ATOM   1376  N   GLU   276     -18.338  11.598  20.123  1.00 12.89
ATOM   1377  CA  GLU   276     -18.862  12.433  21.202  1.00 14.20
ATOM   1378  CB  GLU   276     -19.034  11.622  22.495  1.00 13.06
ATOM   1379  CG  GLU   276     -20.290  10.754  22.586  1.00 15.26
ATOM   1380  CD  GLU   276     -20.168   9.419  21.866  1.00 15.95
ATOM   1381  OE1 GLU   276     -20.955   8.497  22.196  1.00 16.20
ATOM   1382  OE2 GLU   276     -19.299   9.279  20.976  1.00 14.68
ATOM   1383  C   GLU   276     -17.948  13.628  21.480  1.00 14.15
ATOM   1384  O   GLU   276     -18.424  14.722  21.778  1.00 17.73
ATOM   1385  N   LEU   277     -16.636  13.421  21.398  1.00 14.90
ATOM   1386  CA  LEU   277     -15.692  14.511  21.631  1.00 13.53
ATOM   1387  CB  LEU   277     -14.266  13.990  21.835  1.00 11.63
ATOM   1388  CG  LEU   277     -13.236  15.122  21.966  1.00 10.76
ATOM   1389  CD1 LEU   277     -13.574  15.987  23.186  1.00  9.92
ATOM   1390  CD2 LEU   277     -11.826  14.543  22.091  1.00 10.43
ATOM   1391  C   LEU   277     -15.693  15.488  20.466  1.00 13.16
ATOM   1392  O   LEU   277     -15.638  16.708  20.666  1.00 12.56
ATOM   1393  N   TRP   278     -15.743  14.963  19.246  1.00 14.01
ATOM   1394  CA  TRP   278     -15.761  15.835  18.087  1.00 14.48
ATOM   1395  CB  TRP   278     -15.799  15.024  16.791  1.00 13.89
ATOM   1396  CG  TRP   278     -15.772  15.895  15.573  1.00 12.31
ATOM   1397  CD2 TRP   278     -14.783  16.877  15.251  1.00 12.04
ATOM   1398  CE2 TRP   278     -15.187  17.500  14.048  1.00 13.65
ATOM   1399  CE3 TRP   278     -13.592  17.294  15.865  1.00 12.21
ATOM   1400  CD1 TRP   278     -16.710  15.953  14.577  1.00 12.77
ATOM   1401  NE1 TRP   278     -16.366  16.919  13.658  1.00 12.87
ATOM   1402  CZ2 TRP   278     -14.442  18.521  13.446  1.00 13.23
ATOM   1403  CZ3 TRP   278     -12.852  18.308  15.267  1.00 10.09
ATOM   1404  CH2 TRP   278     -13.280  18.909  14.071  1.00 12.81
ATOM   1405  C   TRP   278     -16.976  16.757  18.160  1.00 15.77
ATOM   1406  O   TRP   278     -16.923  17.903  17.712  1.00 15.48
ATOM   1407  N   ALA   279     -18.073  16.254  18.725  1.00 17.05
ATOM   1408  CA  ALA   279     -19.292  17.049  18.868  1.00 15.22
ATOM   1409  CB  ALA   279     -20.427  16.179  19.417  1.00 16.67
ATOM   1410  C   ALA   279     -19.035  18.224  19.812  1.00 15.59
ATOM   1411  O   ALA   279     -19.616  19.301  19.663  1.00 14.01
ATOM   1412  N   GLU   280     -18.147  18.007  20.774  1.00 12.96
ATOM   1413  CA  GLU   280     -17.798  19.020  21.756  1.00 12.96
ATOM   1414  CB  GLU   280     -17.170  18.339  22.977  1.00 14.13
ATOM   1415  CG  GLU   280     -17.222  19.152  24.243  1.00 15.85
ATOM   1416  CD  GLU   280     -16.435  18.527  25.383  1.00 16.42
ATOM   1417  OE1 GLU   280     -16.543  17.301  25.597  1.00 13.70
ATOM   1418  OE2 GLU   280     -15.718  19.275  26.077  1.00 17.31
ATOM   1419  C   GLU   280     -16.814  20.061  21.206  1.00 12.16
ATOM   1420  O   GLU   280     -16.941  21.258  21.471  1.00 12.28
ATOM   1421  N   LEU   281     -15.841  19.597  20.428  1.00 12.45
ATOM   1422  CA  LEU   281     -14.795  20.466  19.897  1.00 11.71
ATOM   1423  CB  LEU   281     -13.515  19.645  19.695  1.00 11.79
ATOM   1424  CG  LEU   281     -13.007  18.864  20.920  1.00 10.02
ATOM   1425  CD1 LEU   281     -11.750  18.098  20.541  1.00 11.37
ATOM   1426  CD2 LEU   281     -12.728  19.813  22.080  1.00 11.90
ATOM   1427  C   LEU   281     -15.092  21.236  18.619  1.00 13.12
ATOM   1428  O   LEU   281     -14.778  22.425  18.518  1.00 11.74
ATOM   1429  N   GLU   282     -15.690  20.568  17.641  1.00 13.11
ATOM   1430  CA  GLU   282     -15.964  21.213  16.356  1.00 15.70
ATOM   1431  CB  GLU   282     -16.824  20.300  15.469  1.00 14.84
ATOM   1432  CG  GLU   282     -17.203  20.929  14.125  1.00 17.67
ATOM   1433  CD  GLU   282     -17.804  19.930  13.159  1.00 20.04
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ATOM   1434  OE1 GLU   282     -17.116  19.553  12.183  1.00 23.90
ATOM   1435  OE2 GLU   282     -18.960  19.508  13.376  1.00 19.77
ATOM   1436  C   GLU   282     -16.587  22.608  16.406  1.00 15.68
ATOM   1437  O   GLU   282     -16.186  23.489  15.648  1.00 16.18
ATOM   1438  N   PRO   283     -17.567  22.834  17.296  1.00 16.06
ATOM   1439  CD  PRO   283     -18.227  21.881  18.204  1.00 16.33
ATOM   1440  CA  PRO   283     -18.199  24.154  17.377  1.00 15.06
ATOM   1441  CB  PRO   283     -19.280  23.961  18.445  1.00 16.15
ATOM   1442  CG  PRO   283     -19.592  22.496  18.368  1.00 15.82
ATOM   1443  C   PRO   283     -17.243  25.286  17.749  1.00 16.14
ATOM   1444  O   PRO   283     -17.475  26.444  17.398  1.00 16.99
ATOM   1445  N   LYS   284     -16.178  24.955  18.471  1.00 13.45
ATOM   1446  CA  LYS   284     -15.227  25.967  18.903  1.00 12.96
ATOM   1447  CB  LYS   284     -15.186  26.020  20.441  1.00 11.42
ATOM   1448  CG  LYS   284     -15.023  24.658  21.116  1.00 11.54
ATOM   1449  CD  LYS   284     -14.830  24.781  22.636  1.00 12.52
ATOM   1450  CE  LYS   284     -14.677  23.401  23.286  1.00 10.01
ATOM   1451  NZ  LYS   284     -14.215  23.499  24.697  1.00  9.91
ATOM   1452  C   LYS   284     -13.827  25.737  18.347  1.00 13.36
ATOM   1453  O   LYS   284     -12.860  26.306  18.858  1.00 13.78
ATOM   1454  N   TRP   285     -13.719  24.911  17.305  1.00 11.11
ATOM   1455  CA  TRP   285     -12.422  24.616  16.699  1.00 13.03
ATOM   1456  CB  TRP   285     -12.610  23.807  15.411  1.00 11.65
ATOM   1457  CG  TRP   285     -11.357  23.115  14.942  1.00 12.50
ATOM   1458  CD2 TRP   285     -10.713  21.994  15.563  1.00 10.69
ATOM   1459  CE2 TRP   285      -9.588  21.668  14.775  1.00 11.32
ATOM   1460  CE3 TRP   285     -10.979  21.232  16.712  1.00 13.47
ATOM   1461  CD1 TRP   285     -10.612  23.418  13.832  1.00 11.60
ATOM   1462  NE1 TRP   285      -9.550  22.551  13.726  1.00 11.68
ATOM   1463  CZ2 TRP   285      -8.725  20.613  15.097  1.00 10.72
ATOM   1464  CZ3 TRP   285     -10.117  20.177  17.036  1.00 11.46
ATOM   1465  CH2 TRP   285      -9.006  19.881  16.229  1.00 11.19
ATOM   1466  C   TRP   285     -11.657  25.918  16.406  1.00 13.22
ATOM   1467  O   TRP   285     -12.177  26.829  15.762  1.00 12.38
ATOM   1468  N   PRO   286     -10.394  26.002  16.860  1.00 14.24
ATOM   1469  CD  PRO   286      -9.641  24.886  17.469  1.00 14.63
ATOM   1470  CA  PRO   286      -9.527  27.172  16.683  1.00 13.78
ATOM   1471  CB  PRO   286      -8.391  26.891  17.650  1.00 13.57
ATOM   1472  CG  PRO   286      -8.204  25.407  17.460  1.00 15.14
ATOM   1473  C   PRO   286      -9.016  27.394  15.262  1.00 14.32
ATOM   1474  O   PRO   286      -9.101  26.505  14.418  1.00 13.53
ATOM   1475  N   LYS   287      -8.469  28.584  15.020  1.00 15.29
ATOM   1476  CA  LYS   287      -7.922  28.934  13.708  1.00 15.33
ATOM   1477  CB  LYS   287      -7.867  30.454  13.531  1.00 18.21
ATOM   1478  CG  LYS   287      -9.168  31.180  13.782  1.00 21.00
ATOM   1479  CD  LYS   287     -10.233  30.766  12.788  1.00 26.31
ATOM   1480  CE  LYS   287     -11.541  31.491  13.065  1.00 28.79
ATOM   1481  NZ  LYS   287     -12.561  31.178  12.027  1.00 31.54
ATOM   1482  C   LYS   287      -6.508  28.378  13.515  1.00 15.32
ATOM   1483  O   LYS   287      -6.040  28.260  12.373  1.00 12.67
ATOM   1484  N   ALA   288      -5.827  28.046  14.616  1.00 12.14
ATOM   1485  CA  ALA   288      -4.454  27.521  14.531  1.00 12.45
ATOM   1486  CB  ALA   288      -3.487  28.650  14.146  1.00  9.63
ATOM   1487  C   ALA   288      -3.972  26.870  15.823  1.00 12.92
ATOM   1488  O   ALA   288      -4.539  27.097  16.896  1.00 13.57
ATOM   1489  N   PHE   289      -2.897  26.090  15.709  1.00 12.44
ATOM   1490  CA  PHE   289      -2.296  25.385  16.843  1.00 12.16
ATOM   1491  CB  PHE   289      -1.612  26.386  17.776  1.00 13.51
ATOM   1492  CG  PHE   289      -0.748  27.382  17.056  1.00 16.00
ATOM   1493  CD1 PHE   289      -1.192  28.684  16.844  1.00 16.15
ATOM   1494  CD2 PHE   289       0.504  27.012  16.570  1.00 15.27
ATOM   1495  CE1 PHE   289      -0.403  29.609  16.159  1.00 17.14
ATOM   1496  CE2 PHE   289       1.299  27.923  15.885  1.00 16.42
ATOM   1497  CZ  PHE   289       0.844  29.229  15.679  1.00 17.43
ATOM   1498  C   PHE   289      -3.361  24.599  17.597  1.00 12.61
ATOM   1499  O   PHE   289      -3.562  24.781  18.808  1.00 11.40
ATOM   1500  N   TRP   290      -4.023  23.701  16.872  1.00 10.38
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ATOM   1501  CA  TRP   290      -5.103  22.908  17.437  1.00 11.21
ATOM   1502  CB  TRP   290      -5.767  22.052  16.345  1.00 10.21
ATOM   1503  CG  TRP   290      -4.925  20.936  15.859  1.00 11.55
ATOM   1504  CD2 TRP   290      -4.802  19.645  16.461  1.00 11.64
ATOM   1505  CE2 TRP   290      -3.802  18.946  15.751  1.00 10.89
ATOM   1506  CE3 TRP   290      -5.434  19.013  17.541  1.00 10.83
ATOM   1507  CD1 TRP   290      -4.032  20.966  14.829  1.00 13.11
ATOM   1508  NE1 TRP   290      -3.350  19.772  14.757  1.00 12.41
ATOM   1509  CZ2 TRP   290      -3.414  17.642  16.087  1.00  9.98
ATOM   1510  CZ3 TRP   290      -5.048  17.720  17.876  1.00 11.47
ATOM   1511  CH2 TRP   290      -4.045  17.050  17.148  1.00 10.26
ATOM   1512  C   TRP   290      -4.702  22.032  18.621  1.00 12.00
ATOM   1513  O   TRP   290      -5.466  21.915  19.582  1.00 12.42
ATOM   1514  N   ASP   291      -3.511  21.433  18.572  1.00 12.22
ATOM   1515  CA  ASP   291      -3.063  20.573  19.667  1.00 11.88
ATOM   1516  CB  ASP   291      -1.813  19.767  19.260  1.00 15.06
ATOM   1517  CG  ASP   291      -0.723  20.625  18.645  1.00 16.75
ATOM   1518  OD1 ASP   291       0.428  20.153  18.575  1.00 17.79
ATOM   1519  OD2 ASP   291      -1.007  21.759  18.221  1.00 20.72
ATOM   1520  C   ASP   291      -2.823  21.309  20.991  1.00 11.66
ATOM   1521  O   ASP   291      -3.212  20.809  22.046  1.00 10.48
ATOM   1522  N   ASP   292      -2.188  22.480  20.952  1.00  9.42
ATOM   1523  CA  ASP   292      -1.956  23.241  22.184  1.00 12.46
ATOM   1524  CB  ASP   292      -0.964  24.389  21.954  1.00 10.77
ATOM   1525  CG  ASP   292       0.484  23.926  22.017  1.00 12.96
ATOM   1526  OD1 ASP   292       0.715  22.733  22.331  1.00 13.75
ATOM   1527  OD2 ASP   292       1.390  24.746  21.764  1.00 11.54
ATOM   1528  C   ASP   292      -3.275  23.793  22.703  1.00 12.08
ATOM   1529  O   ASP   292      -3.431  24.038  23.909  1.00 10.75
ATOM   1530  N   TRP   293      -4.220  23.978  21.783  1.00 11.95
ATOM   1531  CA  TRP   293      -5.559  24.477  22.111  1.00 11.64
ATOM   1532  CB  TRP   293      -6.306  24.811  20.821  1.00 12.26
ATOM   1533  CG  TRP   293      -7.752  25.151  20.983  1.00 12.43
ATOM   1534  CD2 TRP   293      -8.866  24.283  20.737  1.00 12.25
ATOM   1535  CE2 TRP   293     -10.041  25.036  20.968  1.00 13.17
ATOM   1536  CE3 TRP   293      -8.985  22.941  20.342  1.00 12.77
ATOM   1537  CD1 TRP   293      -8.279  26.357  21.351  1.00 15.02
ATOM   1538  NE1 TRP   293      -9.654  26.297  21.342  1.00 13.61
ATOM   1539  CZ2 TRP   293     -11.322  24.493  20.814  1.00 13.14
ATOM   1540  CZ3 TRP   293     -10.258  22.397  20.189  1.00 12.86
ATOM   1541  CH2 TRP   293     -11.411  23.177  20.424  1.00 15.27
ATOM   1542  C   TRP   293      -6.327  23.412  22.896  1.00 12.09
ATOM   1543  O   TRP   293      -7.048  23.719  23.851  1.00 12.03
ATOM   1544  N   MET   294      -6.181  22.156  22.495  1.00 10.94
ATOM   1545  CA  MET   294      -6.863  21.081  23.211  1.00 12.36
ATOM   1546  CB  MET   294      -6.807  19.775  22.414  1.00 13.21
ATOM   1547  CG  MET   294      -7.896  19.646  21.353  1.00 14.35
ATOM   1548  SD  MET   294      -7.717  18.138  20.407  1.00 20.87
ATOM   1549  CE  MET   294      -8.278  16.916  21.613  1.00 20.27
ATOM   1550  C   MET   294      -6.228  20.865  24.578  1.00 11.87
ATOM   1551  O   MET   294      -6.850  20.289  25.472  1.00 13.41
ATOM   1552  N   ARG   295      -4.992  21.329  24.742  1.00 10.05
ATOM   1553  CA  ARG   295      -4.292  21.171  26.005  1.00 11.64
ATOM   1554  CB  ARG   295      -2.778  21.265  25.789  1.00 11.34
ATOM   1555  CG  ARG   295      -2.182  19.961  25.274  1.00 13.71
ATOM   1556  CD  ARG   295      -0.886  20.163  24.496  1.00 14.69
ATOM   1557  NE  ARG   295      -0.451  18.907  23.886  1.00 15.10
ATOM   1558  CZ  ARG   295       0.371  18.828  22.847  1.00 15.74
ATOM   1559  NH1 ARG   295       0.855  19.932  22.291  1.00 16.82
ATOM   1560  NH2 ARG   295       0.705  17.645  22.355  1.00 18.43
ATOM   1561  C   ARG   295      -4.752  22.163  27.069  1.00 12.00
ATOM   1562  O   ARG   295      -4.438  22.007  28.250  1.00 13.16
ATOM   1563  N   ARG   296      -5.511  23.169  26.653  1.00 11.08
ATOM   1564  CA  ARG   296      -6.029  24.162  27.589  1.00 11.70
ATOM   1565  CB  ARG   296      -6.583  25.368  26.837  1.00 11.79
ATOM   1566  CG  ARG   296      -5.564  26.065  25.976  1.00 16.17
ATOM   1567  CD  ARG   296      -6.192  27.243  25.277  1.00 18.20
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ATOM   1568  NE  ARG   296      -5.238  27.958  24.443  1.00 22.02
ATOM   1569  CZ  ARG   296      -5.565  28.993  23.676  1.00 24.28
ATOM   1570  NH1 ARG   296      -6.824  29.423  23.643  1.00 23.15
ATOM   1571  NH2 ARG   296      -4.638  29.607  22.956  1.00 23.67
ATOM   1572  C   ARG   296      -7.149  23.550  28.432  1.00 12.39
ATOM   1573  O   ARG   296      -7.886  22.670  27.973  1.00 10.87
ATOM   1574  N   PRO   297      -7.307  24.024  29.674  1.00 11.94
ATOM   1575  CD  PRO   297      -6.506  25.023  30.407  1.00 11.39
ATOM   1576  CA  PRO   297      -8.370  23.459  30.513  1.00 12.81
ATOM   1577  CB  PRO   297      -8.121  24.108  31.880  1.00 10.17
ATOM   1578  CG  PRO   297      -7.437  25.419  31.534  1.00 11.42
ATOM   1579  C   PRO   297      -9.787  23.692  29.976  1.00 14.14
ATOM   1580  O   PRO   297     -10.681  22.875  30.210  1.00 13.39
ATOM   1581  N   GLU   298      -9.993  24.788  29.247  1.00 13.66
ATOM   1582  CA  GLU   298     -11.313  25.080  28.694  1.00 13.97
ATOM   1583  CB  GLU   298     -11.303  26.391  27.893  1.00 16.73
ATOM   1584  CG  GLU   298     -11.035  27.655  28.700  1.00 20.66
ATOM   1585  CD  GLU   298      -9.631  27.697  29.280  1.00 23.05
ATOM   1586  OE1 GLU   298      -8.694  27.259  28.588  1.00 18.78
ATOM   1587  OE2 GLU   298      -9.467  28.182  30.423  1.00 27.18
ATOM   1588  C   GLU   298     -11.764  23.946  27.773  1.00 13.48
ATOM   1589  O   GLU   298     -12.957  23.721  27.593  1.00 11.08
ATOM   1590  N   GLN   299     -10.801  23.246  27.183  1.00 13.09
ATOM   1591  CA  GLN   299     -11.096  22.134  26.285  1.00 12.70
ATOM   1592  CB  GLN   299     -10.124  22.127  25.103  1.00 13.00
ATOM   1593  CG  GLN   299     -10.478  23.051  23.939  1.00 14.62
ATOM   1594  CD  GLN   299     -10.693  24.495  24.356  1.00 15.61
ATOM   1595  OE1 GLN   299     -11.818  24.905  24.645  1.00 16.24
ATOM   1596  NE2 GLN   299      -9.612  25.274  24.395  1.00 13.25
ATOM   1597  C   GLN   299     -10.981  20.796  27.004  1.00 12.27
ATOM   1598  O   GLN   299     -11.874  19.958  26.922  1.00 10.29
ATOM   1599  N   ARG   300      -9.864  20.608  27.701  1.00 12.36
ATOM   1600  CA  ARG   300      -9.581  19.365  28.414  1.00 13.43
ATOM   1601  CB  ARG   300      -8.181  19.437  29.032  1.00 12.72
ATOM   1602  CG  ARG   300      -7.651  18.103  29.528  1.00 14.33
ATOM   1603  CD  ARG   300      -6.153  18.184  29.817  1.00 15.40
ATOM   1604  NE  ARG   300      -5.842  18.792  31.108  1.00 18.11
ATOM   1605  CZ  ARG   300      -6.070  18.209  32.284  1.00 18.54
ATOM   1606  NH1 ARG   300      -6.618  16.997  32.339  1.00 16.58
ATOM   1607  NH2 ARG   300      -5.737  18.830  33.409  1.00 18.30
ATOM   1608  C   ARG   300     -10.598  19.049  29.497  1.00 12.25
ATOM   1609  O   ARG   300     -11.089  17.925  29.593  1.00 14.49
ATOM   1610  N   LYS   301     -10.890  20.043  30.328  1.00 13.85
ATOM   1611  CA  LYS   301     -11.841  19.877  31.416  1.00 11.99
ATOM   1612  CB  LYS   301     -13.242  19.653  30.843  1.00 12.12
ATOM   1613  CG  LYS   301     -13.810  20.875  30.121  1.00 13.21
ATOM   1614  CD  LYS   301     -15.070  20.535  29.337  1.00 12.52
ATOM   1615  CE  LYS   301     -15.642  21.754  28.628  1.00 17.71
ATOM   1616  NZ  LYS   301     -16.893  21.431  27.868  1.00 18.61
ATOM   1617  C   LYS   301     -11.451  18.723  32.346  1.00 12.92
ATOM   1618  O   LYS   301     -12.258  17.848  32.647  1.00 11.72
ATOM   1619  N   GLY   302     -10.193  18.719  32.773  1.00 12.75
ATOM   1620  CA  GLY   302      -9.713  17.702  33.693  1.00 14.52
ATOM   1621  C   GLY   302      -9.645  16.269  33.202  1.00 14.38
ATOM   1622  O   GLY   302      -9.250  15.380  33.955  1.00 14.72
ATOM   1623  N   ARG   303     -10.005  16.038  31.944  1.00 14.42
ATOM   1624  CA  ARG   303      -9.987  14.693  31.388  1.00 13.60
ATOM   1625  CB  ARG   303     -10.928  14.628  30.184  1.00 14.49
ATOM   1626  CG  ARG   303     -12.400  14.788  30.572  1.00 12.92
ATOM   1627  CD  ARG   303     -13.313  14.924  29.356  1.00 11.58
ATOM   1628  NE  ARG   303     -13.106  16.198  28.676  1.00 13.48
ATOM   1629  CZ  ARG   303     -13.901  16.679  27.721  1.00 13.93
ATOM   1630  NH1 ARG   303     -14.967  15.991  27.322  1.00 12.00
ATOM   1631  NH2 ARG   303     -13.638  17.859  27.178  1.00 13.15
ATOM   1632  C   ARG   303      -8.578  14.252  31.006  1.00 13.39
ATOM   1633  O   ARG   303      -7.700  15.080  30.747  1.00 12.74
ATOM   1634  N   ALA   304      -8.368  12.942  30.984  1.00 12.28
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ATOM	1635	CA	ALA	304	-7.064	12.376	30.663	1.00	12.63
ATOM	1636	CB	ALA	304	-6.530	11.610	31.875	1.00	10.41
ATOM	1637	C	ALA	304	-7.088	11.451	29.453	1.00	10.93
ATOM	1638	O	ALA	304	-8.149	11.114	28.921	1.00	10.47
ATOM	1639	N	CYS	305	-5.901	11.056	29.008	1.00	11.71
ATOM	1640	CA	CYS	305	-5.781	10.123	27.897	1.00	12.01
ATOM	1641	C	CYS	305	-4.988	8.947	28.428	1.00	11.03
ATOM	1642	O	CYS	305	-4.309	9.046	29.446	1.00	10.45
ATOM	1643	CB	CYS	305	-4.948	10.669	26.726	1.00	13.39
ATOM	1644	SG	CYS	305	-5.483	12.076	25.701	1.00	16.95
ATOM	1645	N	VAL	306	-5.064	7.837	27.717	1.00	10.01
ATOM	1646	CA	VAL	306	-4.280	6.675	28.078	1.00	10.46
ATOM	1647	CB	VAL	306	-5.009	5.354	27.727	1.00	7.76
ATOM	1648	CG1	VAL	306	-4.037	4.181	27.816	1.00	8.58
ATOM	1649	CG2	VAL	306	-6.175	5.136	28.692	1.00	10.52
ATOM	1650	C	VAL	306	-3.069	6.822	27.175	1.00	9.51
ATOM	1651	O	VAL	306	-3.196	7.288	26.042	1.00	11.16
ATOM	1652	N	ARG	307	-1.895	6.478	27.688	1.00	9.55
ATOM	1653	CA	ARG	307	-0.667	6.523	26.899	1.00	8.03
ATOM	1654	CB	ARG	307	0.089	7.853	27.102	1.00	9.15
ATOM	1655	CG	ARG	307	0.654	8.119	28.491	1.00	10.37
ATOM	1656	CD	ARG	307	2.016	7.466	28.646	1.00	10.04
ATOM	1657	NE	ARG	307	2.610	7.745	29.953	1.00	12.09
ATOM	1658	CZ	ARG	307	3.780	7.255	30.347	1.00	12.31
ATOM	1659	NH1	ARG	307	4.474	6.468	29.529	1.00	8.22
ATOM	1660	NH2	ARG	307	4.242	7.538	31.553	1.00	9.46
ATOM	1661	C	ARG	307	0.133	5.307	27.381	1.00	8.94
ATOM	1662	O	ARG	307	-0.033	4.865	28.514	1.00	7.31
ATOM	1663	N	PRO	308	0.994	4.744	26.520	1.00	9.64
ATOM	1664	CD	PRO	308	1.159	5.068	25.089	1.00	9.51
ATOM	1665	CA	PRO	308	1.792	3.568	26.879	1.00	8.29
ATOM	1666	CB	PRO	308	1.844	2.808	25.570	1.00	9.08
ATOM	1667	CG	PRO	308	2.081	3.937	24.588	1.00	10.21
ATOM	1668	C	PRO	308	3.193	3.861	27.384	1.00	8.94
ATOM	1669	O	PRO	308	3.712	4.954	27.185	1.00	5.39
ATOM	1670	N	GLU	309	3.802	2.856	28.011	1.00	7.74
ATOM	1671	CA	GLU	309	5.173	2.956	28.503	1.00	8.55
ATOM	1672	CB	GLU	309	5.536	1.683	29.276	1.00	10.77
ATOM	1673	CG	GLU	309	7.023	1.502	29.632	1.00	9.78
ATOM	1674	CD	GLU	309	7.460	2.314	30.832	1.00	13.10
ATOM	1675	OE1	GLU	309	6.603	2.984	31.444	1.00	14.23
ATOM	1676	OE2	GLU	309	8.667	2.278	31.169	1.00	11.36
ATOM	1677	C	GLU	309	6.092	3.099	27.285	1.00	9.37
ATOM	1678	O	GLU	309	7.064	3.862	27.311	1.00	8.65
ATOM	1679	N	ILE	310	5.781	2.345	26.227	1.00	9.31
ATOM	1680	CA	ILE	310	6.556	2.352	24.981	1.00	8.22
ATOM	1681	CB	ILE	310	7.132	0.939	24.684	1.00	6.15
ATOM	1682	CG2	ILE	310	7.948	0.955	23.394	1.00	8.52
ATOM	1683	CG1	ILE	310	8.000	0.479	25.857	1.00	8.94
ATOM	1684	CD1	ILE	310	8.637	-0.908	25.660	1.00	10.39
ATOM	1685	C	ILE	310	5.611	2.780	23.852	1.00	8.74
ATOM	1686	O	ILE	310	4.557	2.169	23.652	1.00	9.27
ATOM	1687	N	SER	311	5.993	3.824	23.118	1.00	10.21
ATOM	1688	CA	SER	311	5.155	4.377	22.048	1.00	10.60
ATOM	1689	CB	SER	311	5.838	5.597	21.420	1.00	10.80
ATOM	1690	OG	SER	311	6.139	6.580	22.395	1.00	15.82
ATOM	1691	C	SER	311	4.757	3.403	20.938	1.00	11.19
ATOM	1692	O	SER	311	5.528	2.519	20.552	1.00	10.45
ATOM	1693	N	ARG	312	3.540	3.574	20.427	1.00	9.62
ATOM	1694	CA	ARG	312	3.051	2.727	19.347	1.00	9.53
ATOM	1695	CB	ARG	312	1.615	2.276	19.620	1.00	9.09
ATOM	1696	CG	ARG	312	1.559	0.825	20.128	1.00	9.15
ATOM	1697	CD	ARG	312	2.355	0.676	21.430	1.00	9.29
ATOM	1698	NE	ARG	312	2.460	-0.720	21.851	1.00	9.75
ATOM	1699	CZ	ARG	312	2.874	-1.113	23.054	1.00	9.08
ATOM	1700	NH1	ARG	312	3.224	-0.217	23.961	1.00	12.76
ATOM	1701	NH2	ARG	312	2.929	-2.404	23.354	1.00	7.36

ATOM	1702	C	ARG	312	3.163	3.433	18.004	1.00	8.46
ATOM	1703	O	ARG	312	2.684	2.943	16.983	1.00	10.20
ATOM	1704	N	THR	313	3.792	4.604	18.026	1.00	7.44
ATOM	1705	CA	THR	313	4.055	5.375	16.813	1.00	8.92
ATOM	1706	CB	THR	313	3.026	6.490	16.541	1.00	8.96
ATOM	1707	OG1	THR	313	2.913	7.324	17.697	1.00	7.15
ATOM	1708	CG2	THR	313	1.681	5.899	16.170	1.00	5.98
ATOM	1709	C	THR	313	5.394	6.061	17.021	1.00	9.30
ATOM	1710	O	THR	313	5.866	6.195	18.152	1.00	6.91
ATOM	1711	N	MET	314	5.994	6.491	15.920	1.00	10.80
ATOM	1712	CA	MET	314	7.265	7.195	15.941	1.00	12.95
ATOM	1713	CB	MET	314	8.432	6.219	15.747	1.00	15.80
ATOM	1714	CG	MET	314	8.327	5.394	14.466	1.00	21.34
ATOM	1715	SD	MET	314	9.935	5.151	13.698	1.00	30.23
ATOM	1716	CE	MET	314	10.258	6.803	13.115	1.00	26.07
ATOM	1717	C	MET	314	7.172	8.132	14.751	1.00	13.38
ATOM	1718	O	MET	314	6.428	7.860	13.807	1.00	13.15
ATOM	1719	N	THR	315	7.904	9.237	14.784	1.00	12.03
ATOM	1720	CA	THR	315	7.845	10.161	13.668	1.00	13.51
ATOM	1721	CB	THR	315	7.393	11.589	14.113	1.00	13.15
ATOM	1722	OG1	THR	315	7.276	12.435	12.960	1.00	14.43
ATOM	1723	CG2	THR	315	8.390	12.212	15.081	1.00	10.92
ATOM	1724	C	THR	315	9.173	10.257	12.928	1.00	14.80
ATOM	1725	O	THR	315	10.248	10.203	13.529	1.00	14.62
ATOM	1726	N	PHE	316	9.079	10.380	11.610	1.00	16.30
ATOM	1727	CA	PHE	316	10.252	10.515	10.758	1.00	16.69
ATOM	1728	CB	PHE	316	10.365	9.320	9.810	1.00	16.19
ATOM	1729	CG	PHE	316	9.109	9.035	9.031	1.00	15.35
ATOM	1730	CD1	PHE	316	8.207	8.074	9.468	1.00	14.22
ATOM	1731	CD2	PHE	316	8.827	9.739	7.862	1.00	14.92
ATOM	1732	CE1	PHE	316	7.041	7.814	8.756	1.00	15.21
ATOM	1733	CE2	PHE	316	7.661	9.488	7.140	1.00	12.87
ATOM	1734	CZ	PHE	316	6.768	8.524	7.590	1.00	14.78
ATOM	1735	C	PHE	316	10.144	11.823	9.960	1.00	18.05
ATOM	1736	O	PHE	316	10.969	12.108	9.098	1.00	18.44
ATOM	1737	N	GLY	317	9.127	12.621	10.277	1.00	19.96
ATOM	1738	CA	GLY	317	8.913	13.889	9.592	1.00	21.09
ATOM	1739	C	GLY	317	9.855	15.026	9.963	1.00	23.63
ATOM	1740	O	GLY	317	9.444	16.025	10.579	1.00	21.70
ATOM	1741	N	ARG	318	11.121	14.877	9.573	1.00	25.18
ATOM	1742	CA	ARG	318	12.158	15.874	9.831	1.00	26.95
ATOM	1743	CB	ARG	318	13.460	15.450	9.147	1.00	30.76
ATOM	1744	CG	ARG	318	14.022	14.139	9.661	1.00	35.86
ATOM	1745	CD	ARG	318	15.330	13.780	8.968	1.00	38.86
ATOM	1746	NE	ARG	318	16.021	12.690	9.655	1.00	41.36
ATOM	1747	CZ	ARG	318	16.528	12.785	10.881	1.00	43.01
ATOM	1748	NH1	ARG	318	16.422	13.922	11.560	1.00	44.95
ATOM	1749	NH2	ARG	318	17.145	11.747	11.429	1.00	43.63
ATOM	1750	C	ARG	318	11.740	17.240	9.297	1.00	26.49
ATOM	1751	O	ARG	318	11.762	18.244	10.017	1.00	24.42
ATOM	1752	N	LYS	319	11.365	17.255	8.022	1.00	25.71
ATOM	1753	CA	LYS	319	10.931	18.464	7.334	1.00	24.83
ATOM	1754	CB	LYS	319	11.494	18.471	5.905	1.00	26.19
ATOM	1755	CG	LYS	319	10.901	19.517	4.969	1.00	25.31
ATOM	1756	CD	LYS	319	11.286	20.933	5.363	1.00	26.83
ATOM	1757	CE	LYS	319	10.675	21.936	4.400	1.00	25.52
ATOM	1758	NZ	LYS	319	9.188	21.813	4.381	1.00	23.14
ATOM	1759	C	LYS	319	9.407	18.484	7.303	1.00	24.12
ATOM	1760	O	LYS	319	8.774	17.519	6.872	1.00	24.11
ATOM	1761	N	GLY	320	8.825	19.581	7.774	1.00	23.51
ATOM	1762	CA	GLY	320	7.379	19.707	7.788	1.00	22.60
ATOM	1763	C	GLY	320	6.955	21.149	7.970	1.00	23.25
ATOM	1764	O	GLY	320	7.648	22.071	7.522	1.00	21.64
ATOM	1765	N	VAL	321	5.810	21.357	8.612	1.00	22.60
ATOM	1766	CA	VAL	321	5.334	22.712	8.853	1.00	25.69
ATOM	1767	CB	VAL	321	3.908	22.712	9.430	1.00	25.05
ATOM	1768	CG1	VAL	321	3.517	24.114	9.872	1.00	24.72

ATOM	1769	CG2	VAL	321	2.941	22.208	8.382	1.00	25.38
ATOM	1770	C	VAL	321	6.286	23.360	9.847	1.00	28.35
ATOM	1771	O	VAL	321	6.967	24.338	9.524	1.00	28.74
ATOM	1772	N	SER	322	6.336	22.804	11.054	1.00	30.98
ATOM	1773	CA	SER	322	7.221	23.320	12.093	1.00	34.70
ATOM	1774	CB	SER	322	6.992	22.593	13.425	1.00	34.98
ATOM	1775	OG	SER	322	5.641	22.668	13.845	1.00	37.08
ATOM	1776	C	SER	322	8.671	23.107	11.682	1.00	36.21
ATOM	1777	O	SER	322	8.977	22.263	10.832	1.00	36.48
ATOM	1778	N	HIS	323	9.560	23.880	12.294	1.00	37.70
ATOM	1779	CA	HIS	323	10.982	23.754	12.024	1.00	38.78
ATOM	1780	CB	HIS	323	11.733	24.954	12.608	1.00	42.18
ATOM	1781	CG	HIS	323	11.174	26.275	12.177	1.00	45.20
ATOM	1782	CD2	HIS	323	10.775	27.353	12.893	1.00	46.73
ATOM	1783	ND1	HIS	323	10.956	26.593	10.852	1.00	46.51
ATOM	1784	CE1	HIS	323	10.445	27.809	10.772	1.00	47.58
ATOM	1785	NE2	HIS	323	10.325	28.292	11.996	1.00	47.98
ATOM	1786	C	HIS	323	11.419	22.449	12.690	1.00	37.28
ATOM	1787	O	HIS	323	10.729	21.941	13.579	1.00	36.32
ATOM	1788	N	GLY	324	12.555	21.909	12.264	1.00	35.81
ATOM	1789	CA	GLY	324	13.014	20.648	12.817	1.00	34.49
ATOM	1790	C	GLY	324	13.786	20.636	14.127	1.00	32.94
ATOM	1791	O	GLY	324	14.436	19.633	14.426	1.00	33.40
ATOM	1792	N	GLN	325	13.728	21.704	14.920	1.00	30.87
ATOM	1793	CA	GLN	325	14.476	21.700	16.176	1.00	28.41
ATOM	1794	CB	GLN	325	14.646	23.113	16.736	1.00	29.50
ATOM	1795	CG	GLN	325	15.500	23.137	18.004	1.00	32.11
ATOM	1796	CD	GLN	325	16.112	24.498	18.292	1.00	35.37
ATOM	1797	OE1	GLN	325	15.400	25.482	18.508	1.00	36.70
ATOM	1798	NE2	GLN	325	17.442	24.559	18.295	1.00	34.41
ATOM	1799	C	GLN	325	13.847	20.807	17.236	1.00	26.38
ATOM	1800	O	GLN	325	14.535	19.997	17.859	1.00	26.04
ATOM	1801	N	PHE	326	12.546	20.954	17.450	1.00	24.30
ATOM	1802	CA	PHE	326	11.862	20.130	18.432	1.00	22.02
ATOM	1803	CB	PHE	326	10.390	20.540	18.548	1.00	22.92
ATOM	1804	CG	PHE	326	9.644	19.812	19.631	1.00	24.00
ATOM	1805	CD1	PHE	326	10.168	19.731	20.920	1.00	23.97
ATOM	1806	CD2	PHE	326	8.425	19.200	19.365	1.00	23.34
ATOM	1807	CE1	PHE	326	9.494	19.048	21.922	1.00	23.54
ATOM	1808	CE2	PHE	326	7.740	18.514	20.362	1.00	23.65
ATOM	1809	CZ	PHE	326	8.275	18.436	21.644	1.00	24.09
ATOM	1810	C	PHE	326	11.975	18.672	17.998	1.00	21.26
ATOM	1811	O	PHE	326	12.134	17.779	18.833	1.00	20.14
ATOM	1812	N	PHE	327	11.912	18.439	16.689	1.00	18.74
ATOM	1813	CA	PHE	327	12.021	17.088	16.139	1.00	19.81
ATOM	1814	CB	PHE	327	11.647	17.067	14.647	1.00	19.41
ATOM	1815	CG	PHE	327	11.896	15.731	13.980	1.00	21.02
ATOM	1816	CD1	PHE	327	10.868	14.799	13.847	1.00	21.52
ATOM	1817	CD2	PHE	327	13.179	15.379	13.556	1.00	20.33
ATOM	1818	CE1	PHE	327	11.110	13.532	13.306	1.00	22.04
ATOM	1819	CE2	PHE	327	13.439	14.119	13.015	1.00	21.31
ATOM	1820	CZ	PHE	327	12.401	13.189	12.890	1.00	21.75
ATOM	1821	C	PHE	327	13.445	16.555	16.286	1.00	20.18
ATOM	1822	O	PHE	327	13.651	15.368	16.567	1.00	19.04
ATOM	1823	N	ASP	328	14.423	17.435	16.080	1.00	19.53
ATOM	1824	CA	ASP	328	15.827	17.051	16.150	1.00	21.03
ATOM	1825	CB	ASP	328	16.713	18.104	15.469	1.00	22.34
ATOM	1826	CG	ASP	328	16.828	17.892	13.966	1.00	25.38
ATOM	1827	OD1	ASP	328	16.789	16.722	13.519	1.00	24.17
ATOM	1828	OD2	ASP	328	16.983	18.894	13.231	1.00	27.10
ATOM	1829	C	ASP	328	16.358	16.804	17.551	1.00	20.43
ATOM	1830	O	ASP	328	17.241	15.967	17.747	1.00	19.20
ATOM	1831	N	GLN	329	15.828	17.525	18.529	1.00	19.78
ATOM	1832	CA	GLN	329	16.308	17.364	19.892	1.00	21.05
ATOM	1833	CB	GLN	329	16.465	18.730	20.551	1.00	22.04
ATOM	1834	CG	GLN	329	17.525	19.598	19.899	1.00	25.40
ATOM	1835	CD	GLN	329	17.772	20.872	20.670	1.00	26.79

ATOM	1836	OE1	GLN	329	16.866	21.689	20.848	1.00	28.98
ATOM	1837	NE2	GLN	329	19.003	21.050	21.140	1.00	27.88
ATOM	1838	C	GLN	329	15.435	16.475	20.760	1.00	20.00
ATOM	1839	O	GLN	329	15.862	16.038	21.829	1.00	18.97
ATOM	1840	N	HIS	330	14.222	16.186	20.303	1.00	16.95
ATOM	1841	CA	HIS	330	13.341	15.356	21.107	1.00	17.59
ATOM	1842	CB	HIS	330	12.368	16.239	21.884	1.00	17.99
ATOM	1843	CG	HIS	330	11.433	15.468	22.759	1.00	18.94
ATOM	1844	CD2	HIS	330	10.116	15.184	22.625	1.00	18.46
ATOM	1845	ND1	HIS	330	11.846	14.845	23.920	1.00	20.65
ATOM	1846	CE1	HIS	330	10.821	14.209	24.462	1.00	19.98
ATOM	1847	NE2	HIS	330	9.760	14.399	23.695	1.00	19.60
ATOM	1848	C	HIS	330	12.535	14.273	20.391	1.00	16.04
ATOM	1849	O	HIS	330	12.712	13.082	20.657	1.00	15.25
ATOM	1850	N	LEU	331	11.645	14.696	19.498	1.00	15.27
ATOM	1851	CA	LEU	331	10.769	13.778	18.787	1.00	12.44
ATOM	1852	CB	LEU	331	9.923	14.541	17.769	1.00	13.09
ATOM	1853	CG	LEU	331	8.970	15.622	18.294	1.00	14.50
ATOM	1854	CD1	LEU	331	8.301	16.282	17.104	1.00	17.18
ATOM	1855	CD2	LEU	331	7.929	15.026	19.233	1.00	12.82
ATOM	1856	C	LEU	331	11.425	12.591	18.097	1.00	12.07
ATOM	1857	O	LEU	331	10.882	11.487	18.136	1.00	10.26
ATOM	1858	N	LYS	332	12.580	12.809	17.470	1.00	11.22
ATOM	1859	CA	LYS	332	13.261	11.734	16.751	1.00	11.05
ATOM	1860	CB	LYS	332	14.439	12.290	15.923	1.00	13.98
ATOM	1861	CG	LYS	332	15.641	12.785	16.757	1.00	16.97
ATOM	1862	CD	LYS	332	16.818	13.270	15.884	1.00	18.06
ATOM	1863	CE	LYS	332	17.639	12.104	15.352	1.00	20.22
ATOM	1864	NZ	LYS	332	18.858	12.539	14.596	1.00	20.25
ATOM	1865	C	LYS	332	13.776	10.626	17.662	1.00	10.62
ATOM	1866	O	LYS	332	14.087	9.537	17.193	1.00	11.08
ATOM	1867	N	PHE	333	13.862	10.892	18.960	1.00	11.27
ATOM	1868	CA	PHE	333	14.387	9.885	19.879	1.00	11.63
ATOM	1869	CB	PHE	333	15.249	10.562	20.949	1.00	13.25
ATOM	1870	CG	PHE	333	16.438	11.280	20.381	1.00	13.82
ATOM	1871	CD1	PHE	333	16.519	12.669	20.425	1.00	12.49
ATOM	1872	CD2	PHE	333	17.450	10.566	19.739	1.00	14.56
ATOM	1873	CE1	PHE	333	17.590	13.342	19.832	1.00	12.68
ATOM	1874	CE2	PHE	333	18.524	11.225	19.144	1.00	14.73
ATOM	1875	CZ	PHE	333	18.591	12.619	19.190	1.00	12.42
ATOM	1876	C	PHE	333	13.349	8.986	20.535	1.00	11.66
ATOM	1877	O	PHE	333	13.708	8.056	21.259	1.00	8.04
ATOM	1878	N	ILE	334	12.071	9.249	20.269	1.00	10.74
ATOM	1879	CA	ILE	334	11.001	8.441	20.837	1.00	14.83
ATOM	1880	CB	ILE	334	9.635	9.151	20.673	1.00	14.87
ATOM	1881	CG2	ILE	334	8.522	8.329	21.290	1.00	15.24
ATOM	1882	CG1	ILE	334	9.702	10.524	21.347	1.00	18.17
ATOM	1883	CD1	ILE	334	10.149	10.488	22.800	1.00	20.00
ATOM	1884	C	ILE	334	11.004	7.086	20.137	1.00	14.93
ATOM	1885	O	ILE	334	10.793	6.995	18.925	1.00	16.29
ATOM	1886	N	LYS	335	11.255	6.041	20.919	1.00	16.56
ATOM	1887	CA	LYS	335	11.344	4.667	20.433	1.00	17.65
ATOM	1888	CB	LYS	335	12.072	3.826	21.489	1.00	21.66
ATOM	1889	CG	LYS	335	12.113	2.326	21.233	1.00	26.22
ATOM	1890	CD	LYS	335	12.794	1.612	22.398	1.00	29.86
ATOM	1891	CE	LYS	335	12.676	0.098	22.292	1.00	32.21
ATOM	1892	NZ	LYS	335	13.298	-0.439	21.050	1.00	32.69
ATOM	1893	C	LYS	335	10.021	3.992	20.063	1.00	16.23
ATOM	1894	O	LYS	335	9.031	4.077	20.793	1.00	14.37
ATOM	1895	N	LEU	336	10.014	3.309	18.924	1.00	15.68
ATOM	1896	CA	LEU	336	8.819	2.599	18.475	1.00	13.99
ATOM	1897	CB	LEU	336	8.797	2.491	16.946	1.00	15.48
ATOM	1898	CG	LEU	336	7.574	1.796	16.325	1.00	15.45
ATOM	1899	CD1	LEU	336	6.319	2.585	16.663	1.00	12.43
ATOM	1900	CD2	LEU	336	7.735	1.703	14.805	1.00	11.53
ATOM	1901	C	LEU	336	8.790	1.198	19.067	1.00	14.57
ATOM	1902	O	LEU	336	9.781	0.461	18.989	1.00	15.85

ATOM	1903	N	ASN	337	7.660	0.820	19.658	1.00	13.45
ATOM	1904	CA	ASN	337	7.532	-0.515	20.219	1.00	13.56
ATOM	1905	CB	ASN	337	6.180	-0.686	20.911	1.00	12.27
ATOM	1906	CG	ASN	337	6.029	-2.051	21.534	1.00	11.70
ATOM	1907	OD1	ASN	337	6.794	-2.424	22.422	1.00	13.70
ATOM	1908	ND2	ASN	337	5.048	-2.811	21.070	1.00	8.34
ATOM	1909	C	ASN	337	7.668	-1.566	19.118	1.00	15.16
ATOM	1910	O	ASN	337	7.110	-1.413	18.024	1.00	14.01
ATOM	1911	N	GLN	338	8.405	-2.631	19.420	1.00	16.00
ATOM	1912	CA	GLN	338	8.632	-3.714	18.469	1.00	18.40
ATOM	1913	CB	GLN	338	10.133	-3.873	18.204	1.00	21.80
ATOM	1914	CG	GLN	338	10.790	-2.650	17.577	1.00	27.84
ATOM	1915	CD	GLN	338	10.237	-2.328	16.199	1.00	30.49
ATOM	1916	OE1	GLN	338	10.622	-1.333	15.581	1.00	34.98
ATOM	1917	NE2	GLN	338	9.332	-3.171	15.708	1.00	31.59
ATOM	1918	C	GLN	338	8.070	-5.051	18.941	1.00	17.68
ATOM	1919	O	GLN	338	7.896	-5.965	18.142	1.00	18.12
ATOM	1920	N	GLN	339	7.797	-5.176	20.237	1.00	15.91
ATOM	1921	CA	GLN	339	7.266	-6.429	20.767	1.00	15.06
ATOM	1922	CB	GLN	339	7.837	-6.719	22.161	1.00	17.55
ATOM	1923	CG	GLN	339	7.351	-8.045	22.740	1.00	23.56
ATOM	1924	CD	GLN	339	8.007	-8.407	24.062	1.00	27.04
ATOM	1925	OE1	GLN	339	7.674	-9.430	24.670	1.00	30.02
ATOM	1926	NE2	GLN	339	8.943	-7.575	24.515	1.00	26.42
ATOM	1927	C	GLN	339	5.747	-6.369	20.831	1.00	12.85
ATOM	1928	O	GLN	339	5.177	-5.534	21.538	1.00	10.25
ATOM	1929	N	PHE	340	5.100	-7.255	20.079	1.00	11.48
ATOM	1930	CA	PHE	340	3.645	-7.298	20.026	1.00	12.08
ATOM	1931	CB	PHE	340	3.170	-8.281	18.946	1.00	9.28
ATOM	1932	CG	PHE	340	1.685	-8.246	18.716	1.00	9.31
ATOM	1933	CD1	PHE	340	1.146	-7.467	17.698	1.00	10.24
ATOM	1934	CD2	PHE	340	0.821	-8.940	19.557	1.00	11.39
ATOM	1935	CE1	PHE	340	-0.230	-7.373	17.518	1.00	6.53
ATOM	1936	CE2	PHE	340	-0.561	-8.852	19.388	1.00	11.24
ATOM	1937	CZ	PHE	340	-1.086	-8.066	18.367	1.00	12.21
ATOM	1938	C	PHE	340	3.031	-7.710	21.359	1.00	11.13
ATOM	1939	O	PHE	340	3.336	-8.776	21.887	1.00	10.33
ATOM	1940	N	VAL	341	2.158	-6.859	21.889	1.00	10.14
ATOM	1941	CA	VAL	341	1.470	-7.139	23.142	1.00	8.23
ATOM	1942	CB	VAL	341	1.553	-5.940	24.108	1.00	8.60
ATOM	1943	CG1	VAL	341	0.718	-6.220	25.351	1.00	9.57
ATOM	1944	CG2	VAL	341	3.008	-5.667	24.491	1.00	6.68
ATOM	1945	C	VAL	341	-0.005	-7.394	22.807	1.00	9.78
ATOM	1946	O	VAL	341	-0.645	-6.574	22.140	1.00	8.53
ATOM	1947	N	PRO	342	-0.558	-8.541	23.240	1.00	9.04
ATOM	1948	CD	PRO	342	0.076	-9.666	23.958	1.00	8.83
ATOM	1949	CA	PRO	342	-1.968	-8.830	22.948	1.00	9.39
ATOM	1950	CB	PRO	342	-2.054	-10.344	23.146	1.00	8.09
ATOM	1951	CG	PRO	342	-1.130	-10.565	24.306	1.00	6.72
ATOM	1952	C	PRO	342	-2.882	-8.067	23.911	1.00	8.13
ATOM	1953	O	PRO	342	-3.560	-8.672	24.741	1.00	10.85
ATOM	1954	N	PHE	343	-2.894	-6.741	23.797	1.00	9.12
ATOM	1955	CA	PHE	343	-3.718	-5.912	24.673	1.00	7.59
ATOM	1956	CB	PHE	343	-3.718	-4.449	24.219	1.00	8.06
ATOM	1957	CG	PHE	343	-2.415	-3.730	24.457	1.00	8.42
ATOM	1958	CD1	PHE	343	-1.536	-3.489	23.407	1.00	8.61
ATOM	1959	CD2	PHE	343	-2.097	-3.246	25.719	1.00	8.45
ATOM	1960	CE1	PHE	343	-0.361	-2.769	23.610	1.00	10.26
ATOM	1961	CE2	PHE	343	-0.926	-2.527	25.934	1.00	11.12
ATOM	1962	CZ	PHE	343	-0.057	-2.286	24.879	1.00	8.23
ATOM	1963	C	PHE	343	-5.155	-6.381	24.790	1.00	8.86
ATOM	1964	O	PHE	343	-5.745	-6.268	25.864	1.00	7.27
ATOM	1965	N	THR	344	-5.729	-6.898	23.704	1.00	7.66
ATOM	1966	CA	THR	344	-7.116	-7.371	23.765	1.00	9.84
ATOM	1967	CB	THR	344	-7.683	-7.745	22.356	1.00	9.23
ATOM	1968	OG1	THR	344	-6.940	-8.831	21.792	1.00	13.57
ATOM	1969	CG2	THR	344	-7.618	-6.543	21.415	1.00	10.48

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ATOM   1970  C   THR   344      -7.287  -8.565  24.714  1.00 11.65
ATOM   1971  O   THR   344      -8.412  -8.895  25.099  1.00 11.47
ATOM   1972  N   GLN   345      -6.181  -9.196  25.111  1.00 12.12
ATOM   1973  CA  GLN   345      -6.245 -10.343  26.028  1.00 10.51
ATOM   1974  CB  GLN   345      -5.275 -11.448  25.594  1.00 11.93
ATOM   1975  CG  GLN   345      -5.507 -12.047  24.200  1.00 12.06
ATOM   1976  CD  GLN   345      -4.459 -13.101  23.858  1.00 14.91
ATOM   1977  OE1 GLN   345      -3.392 -13.142  24.470  1.00 14.13
ATOM   1978  NE2 GLN   345      -4.753 -13.948  22.868  1.00 13.42
ATOM   1979  C   GLN   345      -5.909  -9.962  27.476  1.00 12.38
ATOM   1980  O   GLN   345      -5.930 -10.811  28.365  1.00 11.37
ATOM   1981  N   LEU   346      -5.602  -8.693  27.714  1.00 12.02
ATOM   1982  CA  LEU   346      -5.232  -8.237  29.054  1.00 12.56
ATOM   1983  CB  LEU   346      -4.066  -7.255  28.950  1.00 12.83
ATOM   1984  CG  LEU   346      -2.901  -7.749  28.091  1.00 13.46
ATOM   1985  CD1 LEU   346      -1.817  -6.677  28.003  1.00 13.04
ATOM   1986  CD2 LEU   346      -2.345  -9.020  28.697  1.00 11.61
ATOM   1987  C   LEU   346      -6.363  -7.562  29.816  1.00 12.63
ATOM   1988  O   LEU   346      -7.334  -7.098  29.221  1.00 14.12
ATOM   1989  N   ASP   347      -6.222  -7.488  31.135  1.00 11.65
ATOM   1990  CA  ASP   347      -7.225  -6.838  31.971  1.00 12.05
ATOM   1991  CB  ASP   347      -7.291  -7.507  33.348  1.00 12.62
ATOM   1992  CG  ASP   347      -8.392  -6.932  34.227  1.00 17.47
ATOM   1993  OD1 ASP   347      -8.809  -5.775  33.988  1.00 15.47
ATOM   1994  OD2 ASP   347      -8.833  -7.640  35.166  1.00 17.76
ATOM   1995  C   ASP   347      -6.777  -5.383  32.132  1.00 12.36
ATOM   1996  O   ASP   347      -5.855  -5.098  32.893  1.00 10.53
ATOM   1997  N   LEU   348      -7.416  -4.465  31.409  1.00 11.71
ATOM   1998  CA  LEU   348      -7.042  -3.059  31.493  1.00 13.89
ATOM   1999  CB  LEU   348      -7.054  -2.432  30.091  1.00 14.94
ATOM   2000  CG  LEU   348      -6.170  -3.138  29.058  1.00 13.92
ATOM   2001  CD1 LEU   348      -6.224  -2.383  27.722  1.00 14.21
ATOM   2002  CD2 LEU   348      -4.744  -3.225  29.589  1.00 13.88
ATOM   2003  C   LEU   348      -7.946  -2.248  32.420  1.00 15.18
ATOM   2004  O   LEU   348      -8.057  -1.031  32.274  1.00 13.11
ATOM   2005  N   SER   349      -8.585  -2.916  33.376  1.00 16.21
ATOM   2006  CA  SER   349      -9.478  -2.220  34.301  1.00 16.42
ATOM   2007  CB  SER   349     -10.316  -3.228  35.098  1.00 16.72
ATOM   2008  OG  SER   349      -9.500  -4.040  35.919  1.00 17.34
ATOM   2009  C   SER   349      -8.720  -1.314  35.265  1.00 16.18
ATOM   2010  O   SER   349      -9.318  -0.470  35.933  1.00 17.65
ATOM   2011  N   TYR   350      -7.407  -1.489  35.343  1.00 15.16
ATOM   2012  CA  TYR   350      -6.596  -0.669  36.241  1.00 13.97
ATOM   2013  CB  TYR   350      -5.194  -1.283  36.395  1.00 11.76
ATOM   2014  CG  TYR   350      -4.329  -1.246  35.152  1.00 10.07
ATOM   2015  CD1 TYR   350      -3.396  -0.222  34.952  1.00  9.09
ATOM   2016  CE1 TYR   350      -2.572  -0.203  33.824  1.00  9.56
ATOM   2017  CD2 TYR   350      -4.422  -2.246  34.184  1.00 11.42
ATOM   2018  CE2 TYR   350      -3.605  -2.232  33.043  1.00 11.89
ATOM   2019  CZ  TYR   350      -2.683  -1.212  32.874  1.00 12.14
ATOM   2020  OH  TYR   350      -1.861  -1.218  31.768  1.00 14.92
ATOM   2021  C   TYR   350      -6.498   0.777  35.749  1.00 14.51
ATOM   2022  O   TYR   350      -6.085   1.667  36.502  1.00 13.04
ATOM   2023  N   LEU   351      -6.888   1.006  34.493  1.00 11.49
ATOM   2024  CA  LEU   351      -6.849   2.340  33.903  1.00 12.89
ATOM   2025  CB  LEU   351      -6.661   2.244  32.385  1.00 14.30
ATOM   2026  CG  LEU   351      -5.281   1.798  31.895  1.00 16.48
ATOM   2027  CD1 LEU   351      -5.314   1.604  30.379  1.00 15.82
ATOM   2028  CD2 LEU   351      -4.236   2.853  32.277  1.00 15.13
ATOM   2029  C   LEU   351      -8.091   3.178  34.205  1.00 14.11
ATOM   2030  O   LEU   351      -8.103   4.386  33.962  1.00 14.54
ATOM   2031  N   GLN   352      -9.141   2.539  34.708  1.00 15.53
ATOM   2032  CA  GLN   352     -10.362   3.256  35.053  1.00 17.91
ATOM   2033  CB  GLN   352     -11.454   2.283  35.492  1.00 20.81
ATOM   2034  CG  GLN   352     -11.938   1.340  34.409  1.00 24.90
ATOM   2035  CD  GLN   352     -12.821   0.238  34.966  1.00 28.52
ATOM   2036  OE1 GLN   352     -13.420  -0.535  34.214  1.00 29.50
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ATOM	2037	NE2	GLN	352	-12.902	0.155	36.293	1.00	28.59
ATOM	2038	C	GLN	352	-10.038	4.201	36.201	1.00	16.90
ATOM	2039	O	GLN	352	-9.319	3.840	37.137	1.00	15.67
ATOM	2040	N	GLN	353	-10.586	5.408	36.120	1.00	16.65
ATOM	2041	CA	GLN	353	-10.372	6.458	37.108	1.00	17.13
ATOM	2042	CB	GLN	353	-11.352	7.594	36.828	1.00	18.58
ATOM	2043	CG	GLN	353	-11.403	8.673	37.874	1.00	20.96
ATOM	2044	CD	GLN	353	-12.326	9.804	37.467	1.00	21.62
ATOM	2045	OE1	GLN	353	-13.482	9.578	37.087	1.00	21.65
ATOM	2046	NE2	GLN	353	-11.823	11.025	37.539	1.00	20.97
ATOM	2047	C	GLN	353	-10.448	6.060	38.582	1.00	15.38
ATOM	2048	O	GLN	353	-9.549	6.393	39.362	1.00	13.66
ATOM	2049	N	GLU	354	-11.504	5.351	38.972	1.00	16.29
ATOM	2050	CA	GLU	354	-11.659	4.968	40.374	1.00	17.64
ATOM	2051	CB	GLU	354	-13.061	4.392	40.641	1.00	20.52
ATOM	2052	CG	GLU	354	-13.383	3.059	39.970	1.00	23.56
ATOM	2053	CD	GLU	354	-13.821	3.206	38.524	1.00	25.64
ATOM	2054	OE1	GLU	354	-14.327	2.212	37.957	1.00	28.04
ATOM	2055	OE2	GLU	354	-13.658	4.308	37.955	1.00	26.25
ATOM	2056	C	GLU	354	-10.600	4.004	40.887	1.00	17.29
ATOM	2057	O	GLU	354	-10.398	3.890	42.099	1.00	18.78
ATOM	2058	N	ALA	355	-9.918	3.307	39.984	1.00	15.83
ATOM	2059	CA	ALA	355	-8.871	2.380	40.410	1.00	14.09
ATOM	2060	CB	ALA	355	-8.868	1.140	39.516	1.00	15.06
ATOM	2061	C	ALA	355	-7.506	3.079	40.348	1.00	13.66
ATOM	2062	O	ALA	355	-6.745	3.083	41.318	1.00	12.57
ATOM	2063	N	TYR	356	-7.217	3.677	39.198	1.00	11.22
ATOM	2064	CA	TYR	356	-5.957	4.373	38.972	1.00	13.11
ATOM	2065	CB	TYR	356	-5.976	5.020	37.587	1.00	10.93
ATOM	2066	CG	TYR	356	-4.610	5.279	37.011	1.00	12.34
ATOM	2067	CD1	TYR	356	-3.907	4.264	36.364	1.00	11.84
ATOM	2068	CE1	TYR	356	-2.657	4.495	35.809	1.00	11.02
ATOM	2069	CD2	TYR	356	-4.022	6.542	37.096	1.00	12.96
ATOM	2070	CE2	TYR	356	-2.770	6.785	36.546	1.00	11.62
ATOM	2071	CZ	TYR	356	-2.095	5.751	35.902	1.00	11.24
ATOM	2072	OH	TYR	356	-0.861	5.969	35.348	1.00	10.75
ATOM	2073	C	TYR	356	-5.648	5.442	40.026	1.00	13.31
ATOM	2074	O	TYR	356	-4.568	5.439	40.614	1.00	12.91
ATOM	2075	N	ASP	357	-6.596	6.348	40.261	1.00	13.99
ATOM	2076	CA	ASP	357	-6.416	7.434	41.228	1.00	18.58
ATOM	2077	CB	ASP	357	-7.564	8.443	41.103	1.00	17.58
ATOM	2078	CG	ASP	357	-7.493	9.245	39.816	1.00	18.53
ATOM	2079	OD1	ASP	357	-6.711	8.860	38.919	1.00	18.23
ATOM	2080	OD2	ASP	357	-8.221	10.257	39.694	1.00	18.57
ATOM	2081	C	ASP	357	-6.278	6.981	42.680	1.00	20.21
ATOM	2082	O	ASP	357	-5.933	7.773	43.558	1.00	24.05
ATOM	2083	N	ARG	358	-6.557	5.713	42.941	1.00	20.59
ATOM	2084	CA	ARG	358	-6.410	5.192	44.287	1.00	21.72
ATOM	2085	CB	ARG	358	-7.586	4.272	44.639	1.00	23.57
ATOM	2086	CG	ARG	358	-7.517	3.710	46.045	1.00	29.23
ATOM	2087	CD	ARG	358	-7.152	2.231	46.051	1.00	32.94
ATOM	2088	NE	ARG	358	-8.320	1.366	45.885	1.00	34.91
ATOM	2089	CZ	ARG	358	-8.285	0.036	45.931	1.00	37.07
ATOM	2090	NH1	ARG	358	-7.134	-0.597	46.132	1.00	37.92
ATOM	2091	NH2	ARG	358	-9.404	-0.664	45.796	1.00	36.22
ATOM	2092	C	ARG	358	-5.103	4.410	44.336	1.00	19.97
ATOM	2093	O	ARG	358	-4.219	4.695	45.153	1.00	18.77
ATOM	2094	N	ASP	359	-4.972	3.449	43.424	1.00	18.48
ATOM	2095	CA	ASP	359	-3.796	2.594	43.369	1.00	18.39
ATOM	2096	CB	ASP	359	-4.096	1.360	42.518	1.00	20.64
ATOM	2097	CG	ASP	359	-5.262	0.549	43.058	1.00	23.25
ATOM	2098	OD1	ASP	359	-5.634	0.741	44.239	1.00	23.27
ATOM	2099	OD2	ASP	359	-5.799	-0.293	42.306	1.00	25.73
ATOM	2100	C	ASP	359	-2.503	3.252	42.881	1.00	18.19
ATOM	2101	O	ASP	359	-1.504	3.253	43.600	1.00	17.62
ATOM	2102	N	PHE	360	-2.510	3.814	41.676	1.00	17.37
ATOM	2103	CA	PHE	360	-1.296	4.428	41.152	1.00	16.97

ATOM	2104	CB	PHE	360	-1.512	4.986	39.744	1.00	17.07
ATOM	2105	CG	PHE	360	-0.231	5.402	39.067	1.00	18.10
ATOM	2106	CD1	PHE	360	0.677	4.443	38.625	1.00	18.80
ATOM	2107	CD2	PHE	360	0.096	6.747	38.931	1.00	16.62
ATOM	2108	CE1	PHE	360	1.898	4.817	38.060	1.00	17.33
ATOM	2109	CE2	PHE	360	1.313	7.139	38.367	1.00	17.03
ATOM	2110	CZ	PHE	360	2.217	6.176	37.932	1.00	18.56
ATOM	2111	C	PHE	360	-0.755	5.539	42.049	1.00	16.27
ATOM	2112	O	PHE	360	0.442	5.592	42.317	1.00	14.42
ATOM	2113	N	LEU	361	-1.633	6.427	42.505	1.00	17.30
ATOM	2114	CA	LEU	361	-1.229	7.534	43.378	1.00	16.66
ATOM	2115	CB	LEU	361	-2.418	8.470	43.641	1.00	18.29
ATOM	2116	CG	LEU	361	-2.829	9.407	42.500	1.00	22.36
ATOM	2117	CD1	LEU	361	-1.654	10.321	42.167	1.00	23.96
ATOM	2118	CD2	LEU	361	-3.239	8.608	41.271	1.00	23.13
ATOM	2119	C	LEU	361	-0.674	7.025	44.705	1.00	16.01
ATOM	2120	O	LEU	361	0.278	7.587	45.254	1.00	14.37
ATOM	2121	N	ALA	362	-1.272	5.963	45.226	1.00	15.64
ATOM	2122	CA	ALA	362	-0.798	5.387	46.479	1.00	15.85
ATOM	2123	CB	ALA	362	-1.741	4.272	46.949	1.00	13.61
ATOM	2124	C	ALA	362	0.597	4.830	46.210	1.00	15.17
ATOM	2125	O	ALA	362	1.505	4.962	47.027	1.00	15.56
ATOM	2126	N	ARG	363	0.759	4.224	45.041	1.00	14.64
ATOM	2127	CA	ARG	363	2.038	3.656	44.635	1.00	14.47
ATOM	2128	CB	ARG	363	1.908	3.041	43.236	1.00	17.23
ATOM	2129	CG	ARG	363	3.096	2.198	42.835	1.00	21.12
ATOM	2130	CD	ARG	363	3.207	2.034	41.320	1.00	20.99
ATOM	2131	NE	ARG	363	4.293	1.118	40.989	1.00	23.40
ATOM	2132	CZ	ARG	363	4.206	-0.208	41.055	1.00	21.98
ATOM	2133	NH1	ARG	363	3.073	-0.785	41.429	1.00	20.66
ATOM	2134	NH2	ARG	363	5.262	-0.958	40.766	1.00	21.88
ATOM	2135	C	ARG	363	3.107	4.753	44.612	1.00	13.64
ATOM	2136	O	ARG	363	4.186	4.602	45.184	1.00	12.78
ATOM	2137	N	VAL	364	2.778	5.862	43.954	1.00	12.74
ATOM	2138	CA	VAL	364	3.676	7.008	43.812	1.00	11.88
ATOM	2139	CB	VAL	364	3.045	8.083	42.888	1.00	10.80
ATOM	2140	CG1	VAL	364	3.877	9.381	42.913	1.00	8.02
ATOM	2141	CG2	VAL	364	2.951	7.549	41.484	1.00	8.66
ATOM	2142	C	VAL	364	4.063	7.663	45.136	1.00	13.72
ATOM	2143	O	VAL	364	5.247	7.914	45.385	1.00	13.54
ATOM	2144	N	TYR	365	3.077	7.952	45.980	1.00	13.83
ATOM	2145	CA	TYR	365	3.378	8.592	47.251	1.00	14.12
ATOM	2146	CB	TYR	365	2.219	9.502	47.669	1.00	14.69
ATOM	2147	CG	TYR	365	2.136	10.729	46.787	1.00	15.76
ATOM	2148	CD1	TYR	365	1.372	10.729	45.618	1.00	17.00
ATOM	2149	CE1	TYR	365	1.378	11.826	44.750	1.00	15.24
ATOM	2150	CD2	TYR	365	2.900	11.857	47.071	1.00	17.03
ATOM	2151	CE2	TYR	365	2.918	12.958	46.212	1.00	14.66
ATOM	2152	CZ	TYR	365	2.158	12.936	45.056	1.00	14.44
ATOM	2153	OH	TYR	365	2.199	14.019	44.204	1.00	12.34
ATOM	2154	C	TYR	365	3.758	7.624	48.362	1.00	14.74
ATOM	2155	O	TYR	365	4.032	8.034	49.496	1.00	16.61
ATOM	2156	N	GLY	366	3.784	6.341	48.025	1.00	14.23
ATOM	2157	CA	GLY	366	4.183	5.323	48.979	1.00	17.95
ATOM	2158	C	GLY	366	5.646	4.994	48.717	1.00	18.14
ATOM	2159	O	GLY	366	6.341	4.440	49.566	1.00	18.62
ATOM	2160	N	ALA	367	6.114	5.352	47.524	1.00	19.27
ATOM	2161	CA	ALA	367	7.496	5.104	47.138	1.00	19.30
ATOM	2162	CB	ALA	367	7.667	5.329	45.638	1.00	19.88
ATOM	2163	C	ALA	367	8.430	6.023	47.913	1.00	19.59
ATOM	2164	O	ALA	367	8.090	7.171	48.210	1.00	19.14
ATOM	2165	N	PRO	368	9.630	5.533	48.247	1.00	19.84
ATOM	2166	CD	PRO	368	10.235	4.232	47.906	1.00	21.38
ATOM	2167	CA	PRO	368	10.571	6.366	48.989	1.00	19.64
ATOM	2168	CB	PRO	368	11.716	5.401	49.288	1.00	19.41
ATOM	2169	CG	PRO	368	11.713	4.510	48.100	1.00	21.70
ATOM	2170	C	PRO	368	11.019	7.578	48.180	1.00	20.14

ATOM	2171	O	PRO	368	11.092	7.533	46.953	1.00	18.58
ATOM	2172	N	GLN	369	11.311	8.664	48.883	1.00	21.56
ATOM	2173	CA	GLN	369	11.761	9.897	48.251	1.00	21.89
ATOM	2174	CB	GLN	369	11.321	11.089	49.097	1.00	22.69
ATOM	2175	CG	GLN	369	11.319	12.416	48.366	1.00	26.31
ATOM	2176	CD	GLN	369	10.649	13.514	49.173	1.00	28.51
ATOM	2177	OE1	GLN	369	9.536	13.337	49.685	1.00	28.42
ATOM	2178	NE2	GLN	369	11.316	14.658	49.285	1.00	27.64
ATOM	2179	C	GLN	369	13.284	9.857	48.156	1.00	21.25
ATOM	2180	O	GLN	369	13.950	9.397	49.079	1.00	20.74
ATOM	2181	N	LEU	370	13.835	10.319	47.040	1.00	21.53
ATOM	2182	CA	LEU	370	15.283	10.326	46.867	1.00	21.41
ATOM	2183	CB	LEU	370	15.725	9.147	45.983	1.00	21.00
ATOM	2184	CG	LEU	370	17.230	8.857	45.913	1.00	18.83
ATOM	2185	CD1	LEU	370	17.733	8.476	47.305	1.00	19.34
ATOM	2186	CD2	LEU	370	17.514	7.731	44.927	1.00	20.12
ATOM	2187	C	LEU	370	15.735	11.646	46.242	1.00	22.02
ATOM	2188	O	LEU	370	15.082	12.177	45.336	1.00	21.53
ATOM	2189	N	GLN	371	16.847	12.177	46.742	1.00	22.13
ATOM	2190	CA	GLN	371	17.398	13.429	46.232	1.00	22.35
ATOM	2191	CB	GLN	371	18.680	13.777	46.988	1.00	25.11
ATOM	2192	CG	GLN	371	18.445	14.269	48.398	1.00	30.35
ATOM	2193	CD	GLN	371	19.581	13.908	49.329	1.00	34.45
ATOM	2194	OE1	GLN	371	20.757	14.055	48.982	1.00	37.23
ATOM	2195	NE2	GLN	371	19.239	13.436	50.526	1.00	35.47
ATOM	2196	C	GLN	371	17.702	13.275	44.751	1.00	21.70
ATOM	2197	O	GLN	371	18.297	12.283	44.341	1.00	19.79
ATOM	2198	N	VAL	372	17.300	14.255	43.949	1.00	20.48
ATOM	2199	CA	VAL	372	17.535	14.190	42.510	1.00	21.07
ATOM	2200	CB	VAL	372	17.172	15.535	41.827	1.00	20.95
ATOM	2201	CG1	VAL	372	18.048	16.656	42.368	1.00	21.03
ATOM	2202	CG2	VAL	372	17.310	15.409	40.318	1.00	17.84
ATOM	2203	C	VAL	372	18.979	13.808	42.160	1.00	21.88
ATOM	2204	O	VAL	372	19.219	12.997	41.261	1.00	22.02
ATOM	2205	N	GLU	373	19.935	14.377	42.885	1.00	22.91
ATOM	2206	CA	GLU	373	21.349	14.105	42.645	1.00	23.34
ATOM	2207	CB	GLU	373	22.203	14.970	43.579	1.00	26.39
ATOM	2208	CG	GLU	373	23.697	14.967	43.283	1.00	31.49
ATOM	2209	CD	GLU	373	24.025	15.460	41.881	1.00	34.48
ATOM	2210	OE1	GLU	373	23.366	16.417	41.412	1.00	35.50
ATOM	2211	OE2	GLU	373	24.950	14.898	41.252	1.00	35.07
ATOM	2212	C	GLU	373	21.684	12.626	42.850	1.00	21.93
ATOM	2213	O	GLU	373	22.500	12.062	42.129	1.00	18.23
ATOM	2214	N	LYS	374	21.059	12.002	43.844	1.00	19.99
ATOM	2215	CA	LYS	374	21.310	10.596	44.104	1.00	20.27
ATOM	2216	CB	LYS	374	20.674	10.191	45.435	1.00	20.91
ATOM	2217	CG	LYS	374	21.349	10.823	46.643	1.00	22.90
ATOM	2218	CD	LYS	374	20.752	10.309	47.940	1.00	25.08
ATOM	2219	CE	LYS	374	21.498	10.861	49.143	1.00	28.06
ATOM	2220	NZ	LYS	374	20.932	10.338	50.426	1.00	30.10
ATOM	2221	C	LYS	374	20.782	9.726	42.961	1.00	20.03
ATOM	2222	O	LYS	374	21.365	8.683	42.636	1.00	19.27
ATOM	2223	N	VAL	375	19.689	10.164	42.341	1.00	18.52
ATOM	2224	CA	VAL	375	19.093	9.427	41.229	1.00	19.54
ATOM	2225	CB	VAL	375	17.690	9.982	40.860	1.00	19.12
ATOM	2226	CG1	VAL	375	17.135	9.233	39.654	1.00	19.09
ATOM	2227	CG2	VAL	375	16.744	9.861	42.041	1.00	17.13
ATOM	2228	C	VAL	375	19.980	9.536	39.989	1.00	21.78
ATOM	2229	O	VAL	375	20.294	8.535	39.346	1.00	21.25
ATOM	2230	N	ARG	376	20.374	10.766	39.667	1.00	23.27
ATOM	2231	CA	ARG	376	21.203	11.048	38.502	1.00	26.24
ATOM	2232	CB	ARG	376	21.531	12.548	38.432	1.00	27.38
ATOM	2233	CG	ARG	376	22.039	12.976	37.060	1.00	31.67
ATOM	2234	CD	ARG	376	22.975	14.181	37.098	1.00	34.71
ATOM	2235	NE	ARG	376	22.295	15.446	37.363	1.00	36.92
ATOM	2236	CZ	ARG	376	22.859	16.639	37.182	1.00	38.93
ATOM	2237	NH1	ARG	376	24.105	16.721	36.734	1.00	39.86

ATOM	2238	NH2	ARG	376	22.185	17.750	37.451	1.00	39.22
ATOM	2239	C	ARG	376	22.504	10.248	38.474	1.00	25.46
ATOM	2240	O	ARG	376	22.906	9.747	37.424	1.00	26.55
ATOM	2241	N	THR	377	23.157	10.121	39.625	1.00	26.52
ATOM	2242	CA	THR	377	24.424	9.396	39.700	1.00	26.78
ATOM	2243	CB	THR	377	25.344	10.006	40.757	1.00	26.51
ATOM	2244	OG1	THR	377	24.749	9.848	42.051	1.00	26.59
ATOM	2245	CG2	THR	377	25.560	11.483	40.472	1.00	27.45
ATOM	2246	C	THR	377	24.260	7.920	40.022	1.00	26.38
ATOM	2247	O	THR	377	25.244	7.215	40.231	1.00	27.61
ATOM	2248	N	ASN	378	23.018	7.455	40.071	1.00	25.91
ATOM	2249	CA	ASN	378	22.733	6.053	40.356	1.00	25.17
ATOM	2250	CB	ASN	378	23.444	5.151	39.342	1.00	26.24
ATOM	2251	CG	ASN	378	22.491	4.217	38.622	1.00	26.59
ATOM	2252	OD1	ASN	378	21.565	3.671	39.222	1.00	26.43
ATOM	2253	ND2	ASN	378	22.723	4.018	37.329	1.00	29.00
ATOM	2254	C	ASN	378	23.129	5.625	41.770	1.00	24.96
ATOM	2255	O	ASN	378	23.633	4.517	41.972	1.00	24.43
ATOM	2256	N	ASP	379	22.906	6.497	42.746	1.00	24.58
ATOM	2257	CA	ASP	379	23.220	6.167	44.132	1.00	25.43
ATOM	2258	CB	ASP	379	23.570	7.437	44.913	1.00	27.91
ATOM	2259	CG	ASP	379	23.952	7.147	46.352	1.00	31.01
ATOM	2260	OD1	ASP	379	24.789	6.245	46.572	1.00	30.23
ATOM	2261	OD2	ASP	379	23.421	7.823	47.262	1.00	34.67
ATOM	2262	C	ASP	379	22.000	5.478	44.756	1.00	24.99
ATOM	2263	O	ASP	379	20.875	5.640	44.271	1.00	25.33
ATOM	2264	N	ARG	380	22.221	4.698	45.813	1.00	22.28
ATOM	2265	CA	ARG	380	21.130	3.998	46.483	1.00	20.58
ATOM	2266	CB	ARG	380	20.200	5.013	47.152	1.00	20.27
ATOM	2267	CG	ARG	380	20.841	5.814	48.276	1.00	20.83
ATOM	2268	CD	ARG	380	21.104	4.944	49.494	1.00	21.33
ATOM	2269	NE	ARG	380	19.866	4.411	50.058	1.00	21.78
ATOM	2270	CZ	ARG	380	18.913	5.161	50.603	1.00	23.05
ATOM	2271	NH1	ARG	380	19.058	6.478	50.660	1.00	22.04
ATOM	2272	NH2	ARG	380	17.809	4.597	51.083	1.00	24.16
ATOM	2273	C	ARG	380	20.325	3.137	45.502	1.00	19.49
ATOM	2274	O	ARG	380	19.097	3.209	45.460	1.00	19.44
ATOM	2275	N	LYS	381	21.016	2.307	44.729	1.00	18.40
ATOM	2276	CA	LYS	381	20.348	1.469	43.743	1.00	18.63
ATOM	2277	CB	LYS	381	21.393	0.788	42.856	1.00	20.94
ATOM	2278	CG	LYS	381	22.177	1.777	42.011	1.00	23.64
ATOM	2279	CD	LYS	381	23.422	1.164	41.385	1.00	26.26
ATOM	2280	CE	LYS	381	23.085	0.104	40.354	1.00	26.92
ATOM	2281	NZ	LYS	381	24.320	-0.340	39.640	1.00	30.38
ATOM	2282	C	LYS	381	19.375	0.433	44.301	1.00	16.69
ATOM	2283	O	LYS	381	18.599	-0.149	43.545	1.00	14.99
ATOM	2284	N	GLU	382	19.394	0.203	45.612	1.00	15.81
ATOM	2285	CA	GLU	382	18.476	-0.776	46.184	1.00	13.94
ATOM	2286	CB	GLU	382	18.808	-1.076	47.654	1.00	14.67
ATOM	2287	CG	GLU	382	18.586	0.093	48.599	1.00	14.74
ATOM	2288	CD	GLU	382	19.793	0.993	48.700	1.00	12.85
ATOM	2289	OE1	GLU	382	20.602	1.015	47.746	1.00	13.50
ATOM	2290	OE2	GLU	382	19.927	1.686	49.731	1.00	13.80
ATOM	2291	C	GLU	382	17.051	-0.248	46.085	1.00	15.30
ATOM	2292	O	GLU	382	16.094	-0.989	46.304	1.00	14.15
ATOM	2293	N	LEU	383	16.915	1.038	45.761	1.00	14.71
ATOM	2294	CA	LEU	383	15.600	1.659	45.627	1.00	14.26
ATOM	2295	CB	LEU	383	15.646	3.112	46.124	1.00	12.33
ATOM	2296	CG	LEU	383	16.136	3.287	47.564	1.00	13.27
ATOM	2297	CD1	LEU	383	16.305	4.765	47.907	1.00	11.38
ATOM	2298	CD2	LEU	383	15.142	2.611	48.512	1.00	14.31
ATOM	2299	C	LEU	383	15.207	1.606	44.150	1.00	15.23
ATOM	2300	O	LEU	383	15.494	2.531	43.388	1.00	16.80
ATOM	2301	N	GLY	384	14.568	0.505	43.756	1.00	14.85
ATOM	2302	CA	GLY	384	14.151	0.322	42.376	1.00	15.26
ATOM	2303	C	GLY	384	13.045	1.249	41.897	1.00	15.63
ATOM	2304	O	GLY	384	12.812	1.366	40.688	1.00	16.10

ATOM	2305	N	GLU	385	12.361	1.909	42.826	1.00	14.54
ATOM	2306	CA	GLU	385	11.278	2.829	42.465	1.00	12.93
ATOM	2307	CB	GLU	385	9.922	2.109	42.492	1.00	12.53
ATOM	2308	CG	GLU	385	8.755	2.961	41.987	1.00	13.24
ATOM	2309	CD	GLU	385	7.520	2.134	41.651	1.00	13.71
ATOM	2310	OE1	GLU	385	7.642	0.898	41.548	1.00	13.92
ATOM	2311	OE2	GLU	385	6.427	2.715	41.479	1.00	12.55
ATOM	2312	C	GLU	385	11.267	3.991	43.442	1.00	13.04
ATOM	2313	O	GLU	385	10.999	3.818	44.635	1.00	14.12
ATOM	2314	N	VAL	386	11.555	5.184	42.938	1.00	10.99
ATOM	2315	CA	VAL	386	11.593	6.345	43.806	1.00	11.19
ATOM	2316	CB	VAL	386	13.023	6.856	43.980	1.00	12.07
ATOM	2317	CG1	VAL	386	13.907	5.750	44.535	1.00	12.74
ATOM	2318	CG2	VAL	386	13.555	7.362	42.640	1.00	9.26
ATOM	2319	C	VAL	386	10.751	7.506	43.337	1.00	12.56
ATOM	2320	O	VAL	386	10.200	7.515	42.228	1.00	11.44
ATOM	2321	N	ARG	387	10.676	8.498	44.209	1.00	13.41
ATOM	2322	CA	ARG	387	9.939	9.712	43.958	1.00	15.47
ATOM	2323	CB	ARG	387	8.788	9.824	44.967	1.00	17.09
ATOM	2324	CG	ARG	387	7.916	11.055	44.850	1.00	17.92
ATOM	2325	CD	ARG	387	6.561	10.789	45.500	1.00	18.15
ATOM	2326	NE	ARG	387	6.700	10.130	46.800	1.00	23.39
ATOM	2327	CZ	ARG	387	6.961	10.761	47.941	1.00	23.37
ATOM	2328	NH1	ARG	387	7.109	12.077	47.953	1.00	24.71
ATOM	2329	NH2	ARG	387	7.079	10.076	49.070	1.00	22.98
ATOM	2330	C	ARG	387	10.911	10.865	44.136	1.00	16.54
ATOM	2331	O	ARG	387	11.569	10.972	45.166	1.00	18.79
ATOM	2332	N	VAL	388	11.045	11.686	43.102	1.00	16.81
ATOM	2333	CA	VAL	388	11.893	12.871	43.155	1.00	15.82
ATOM	2334	CB	VAL	388	12.738	13.046	41.874	1.00	17.13
ATOM	2335	CG1	VAL	388	13.382	14.442	41.856	1.00	17.34
ATOM	2336	CG2	VAL	388	13.828	11.978	41.825	1.00	15.92
ATOM	2337	C	VAL	388	10.850	13.974	43.252	1.00	17.40
ATOM	2338	O	VAL	388	10.083	14.207	42.313	1.00	16.02
ATOM	2339	N	GLN	389	10.802	14.635	44.400	1.00	16.69
ATOM	2340	CA	GLN	389	9.803	15.672	44.625	1.00	18.37
ATOM	2341	CB	GLN	389	9.383	15.660	46.099	1.00	19.17
ATOM	2342	CG	GLN	389	8.424	16.772	46.509	1.00	22.05
ATOM	2343	CD	GLN	389	7.898	16.587	47.931	1.00	22.87
ATOM	2344	OE1	GLN	389	7.089	15.697	48.195	1.00	24.32
ATOM	2345	NE2	GLN	389	8.367	17.424	48.853	1.00	23.33
ATOM	2346	C	GLN	389	10.246	17.065	44.228	1.00	17.46
ATOM	2347	O	GLN	389	11.344	17.498	44.573	1.00	17.53
ATOM	2348	N	TYR	390	9.388	17.754	43.478	1.00	16.76
ATOM	2349	CA	TYR	390	9.659	19.125	43.064	1.00	17.75
ATOM	2350	CB	TYR	390	9.565	19.273	41.535	1.00	16.18
ATOM	2351	CG	TYR	390	8.182	19.071	40.934	1.00	14.63
ATOM	2352	CD1	TYR	390	7.233	20.106	40.938	1.00	13.62
ATOM	2353	CE1	TYR	390	5.983	19.947	40.337	1.00	14.41
ATOM	2354	CD2	TYR	390	7.839	17.866	40.320	1.00	14.09
ATOM	2355	CE2	TYR	390	6.586	17.691	39.713	1.00	13.66
ATOM	2356	CZ	TYR	390	5.666	18.736	39.721	1.00	15.33
ATOM	2357	OH	TYR	390	4.449	18.576	39.089	1.00	10.47
ATOM	2358	C	TYR	390	8.598	19.964	43.771	1.00	18.49
ATOM	2359	O	TYR	390	7.486	19.491	44.018	1.00	18.13
ATOM	2360	N	THR	391	8.936	21.197	44.116	1.00	18.89
ATOM	2361	CA	THR	391	7.988	22.049	44.818	1.00	21.73
ATOM	2362	CB	THR	391	8.566	22.509	46.174	1.00	20.95
ATOM	2363	OG1	THR	391	9.884	23.032	45.975	1.00	21.00
ATOM	2364	CG2	THR	391	8.631	21.341	47.143	1.00	22.27
ATOM	2365	C	THR	391	7.562	23.270	44.021	1.00	23.03
ATOM	2366	O	THR	391	6.407	23.678	44.072	1.00	26.26
ATOM	2367	N	GLY	392	8.488	23.859	43.281	1.00	23.67
ATOM	2368	CA	GLY	392	8.135	25.027	42.502	1.00	24.37
ATOM	2369	C	GLY	392	8.404	24.826	41.031	1.00	23.92
ATOM	2370	O	GLY	392	8.854	23.762	40.613	1.00	22.74
ATOM	2371	N	ARG	393	8.127	25.854	40.243	1.00	24.20

ATOM	2372	CA	ARG	393	8.353	25.792	38.809	1.00	25.94
ATOM	2373	CB	ARG	393	7.780	27.047	38.143	1.00	28.53
ATOM	2374	CG	ARG	393	8.220	28.360	38.788	1.00	32.90
ATOM	2375	CD	ARG	393	7.388	29.533	38.279	1.00	33.62
ATOM	2376	NE	ARG	393	6.031	29.531	38.823	1.00	37.20
ATOM	2377	CZ	ARG	393	5.031	30.267	38.342	1.00	38.22
ATOM	2378	NH1	ARG	393	5.239	31.063	37.303	1.00	38.98
ATOM	2379	NH2	ARG	393	3.825	30.211	38.896	1.00	35.84
ATOM	2380	C	ARG	393	9.842	25.645	38.502	1.00	24.29
ATOM	2381	O	ARG	393	10.223	24.915	37.594	1.00	24.57
ATOM	2382	N	ASP	394	10.681	26.332	39.270	1.00	25.24
ATOM	2383	CA	ASP	394	12.127	26.261	39.072	1.00	24.22
ATOM	2384	CB	ASP	394	12.846	27.259	39.986	1.00	26.73
ATOM	2385	CG	ASP	394	12.558	28.699	39.619	1.00	29.89
ATOM	2386	OD1	ASP	394	12.684	29.039	38.424	1.00	33.19
ATOM	2387	OD2	ASP	394	12.216	29.494	40.522	1.00	31.70
ATOM	2388	C	ASP	394	12.678	24.859	39.338	1.00	22.40
ATOM	2389	O	ASP	394	13.498	24.351	38.567	1.00	19.93
ATOM	2390	N	SER	395	12.243	24.246	40.437	1.00	19.45
ATOM	2391	CA	SER	395	12.709	22.909	40.775	1.00	20.11
ATOM	2392	CB	SER	395	12.271	22.513	42.198	1.00	20.67
ATOM	2393	OG	SER	395	10.867	22.612	42.384	1.00	24.26
ATOM	2394	C	SER	395	12.206	21.890	39.751	1.00	19.52
ATOM	2395	O	SER	395	12.939	20.970	39.373	1.00	17.21
ATOM	2396	N	PHE	396	10.967	22.047	39.290	1.00	18.02
ATOM	2397	CA	PHE	396	10.447	21.112	38.295	1.00	18.56
ATOM	2398	CB	PHE	396	9.031	21.482	37.843	1.00	17.49
ATOM	2399	CG	PHE	396	8.585	20.723	36.624	1.00	18.20
ATOM	2400	CD1	PHE	396	8.211	19.382	36.718	1.00	17.94
ATOM	2401	CD2	PHE	396	8.624	21.319	35.365	1.00	17.30
ATOM	2402	CE1	PHE	396	7.892	18.646	35.579	1.00	16.48
ATOM	2403	CE2	PHE	396	8.307	20.590	34.223	1.00	17.56
ATOM	2404	CZ	PHE	396	7.941	19.251	34.330	1.00	15.55
ATOM	2405	C	PHE	396	11.344	21.105	37.065	1.00	18.22
ATOM	2406	O	PHE	396	11.828	20.055	36.644	1.00	17.94
ATOM	2407	N	LYS	397	11.565	22.281	36.487	1.00	18.27
ATOM	2408	CA	LYS	397	12.391	22.382	35.288	1.00	21.55
ATOM	2409	CB	LYS	397	12.371	23.816	34.747	1.00	22.89
ATOM	2410	CG	LYS	397	11.230	24.066	33.756	1.00	24.58
ATOM	2411	CD	LYS	397	11.208	25.499	33.266	1.00	26.22
ATOM	2412	CE	LYS	397	10.206	25.671	32.136	1.00	28.79
ATOM	2413	NZ	LYS	397	10.592	24.866	30.936	1.00	30.87
ATOM	2414	C	LYS	397	13.829	21.914	35.476	1.00	21.16
ATOM	2415	O	LYS	397	14.415	21.328	34.567	1.00	21.98
ATOM	2416	N	ALA	398	14.397	22.165	36.648	1.00	21.75
ATOM	2417	CA	ALA	398	15.771	21.750	36.917	1.00	21.39
ATOM	2418	CB	ALA	398	16.270	22.392	38.198	1.00	20.93
ATOM	2419	C	ALA	398	15.861	20.229	37.021	1.00	20.93
ATOM	2420	O	ALA	398	16.698	19.604	36.374	1.00	21.90
ATOM	2421	N	PHE	399	14.989	19.638	37.833	1.00	21.11
ATOM	2422	CA	PHE	399	14.984	18.191	38.015	1.00	20.14
ATOM	2423	CB	PHE	399	13.985	17.798	39.106	1.00	18.69
ATOM	2424	CG	PHE	399	14.299	18.380	40.467	1.00	17.20
ATOM	2425	CD1	PHE	399	13.444	18.160	41.540	1.00	16.46
ATOM	2426	CD2	PHE	399	15.441	19.156	40.669	1.00	16.06
ATOM	2427	CE1	PHE	399	13.715	18.704	42.803	1.00	17.71
ATOM	2428	CE2	PHE	399	15.723	19.702	41.918	1.00	14.40
ATOM	2429	CZ	PHE	399	14.857	19.476	42.990	1.00	16.25
ATOM	2430	C	PHE	399	14.649	17.481	36.702	1.00	21.66
ATOM	2431	O	PHE	399	15.289	16.488	36.346	1.00	22.19
ATOM	2432	N	ALA	400	13.653	17.998	35.983	1.00	20.97
ATOM	2433	CA	ALA	400	13.246	17.426	34.703	1.00	21.06
ATOM	2434	CB	ALA	400	12.117	18.261	34.094	1.00	19.88
ATOM	2435	C	ALA	400	14.439	17.387	33.747	1.00	21.35
ATOM	2436	O	ALA	400	14.742	16.358	33.145	1.00	21.04
ATOM	2437	N	LYS	401	15.111	18.524	33.616	1.00	21.77
ATOM	2438	CA	LYS	401	16.269	18.641	32.744	1.00	23.20

ATOM	2439	CB	LYS	401	16.698	20.112	32.675	1.00	25.09
ATOM	2440	CG	LYS	401	17.903	20.400	31.800	1.00	28.32
ATOM	2441	CD	LYS	401	18.061	21.907	31.610	1.00	30.88
ATOM	2442	CE	LYS	401	19.455	22.270	31.120	1.00	32.77
ATOM	2443	NZ	LYS	401	20.497	21.910	32.129	1.00	32.77
ATOM	2444	C	LYS	401	17.419	17.761	33.246	1.00	22.19
ATOM	2445	O	LYS	401	18.141	17.154	32.458	1.00	23.91
ATOM	2446	N	ALA	402	17.578	17.676	34.559	1.00	22.43
ATOM	2447	CA	ALA	402	18.643	16.864	35.131	1.00	20.91
ATOM	2448	CB	ALA	402	18.708	17.086	36.635	1.00	21.17
ATOM	2449	C	ALA	402	18.473	15.372	34.827	1.00	21.48
ATOM	2450	O	ALA	402	19.458	14.651	34.672	1.00	20.83
ATOM	2451	N	LEU	403	17.230	14.910	34.729	1.00	20.76
ATOM	2452	CA	LEU	403	16.973	13.495	34.463	1.00	22.26
ATOM	2453	CB	LEU	403	15.868	12.987	35.393	1.00	21.72
ATOM	2454	CG	LEU	403	16.148	13.219	36.882	1.00	23.43
ATOM	2455	CD1	LEU	403	14.938	12.835	37.706	1.00	23.46
ATOM	2456	CD2	LEU	403	17.370	12.421	37.308	1.00	23.33
ATOM	2457	C	LEU	403	16.626	13.174	33.005	1.00	21.87
ATOM	2458	O	LEU	403	16.352	12.022	32.670	1.00	22.79
ATOM	2459	N	GLY	404	16.632	14.189	32.146	1.00	21.08
ATOM	2460	CA	GLY	404	16.359	13.967	30.736	1.00	20.52
ATOM	2461	C	GLY	404	14.908	13.922	30.288	1.00	20.04
ATOM	2462	O	GLY	404	14.608	13.403	29.210	1.00	17.90
ATOM	2463	N	VAL	405	14.010	14.460	31.109	1.00	20.50
ATOM	2464	CA	VAL	405	12.587	14.496	30.788	1.00	20.43
ATOM	2465	CB	VAL	405	11.724	14.493	32.079	1.00	21.72
ATOM	2466	CG1	VAL	405	10.260	14.743	31.730	1.00	22.81
ATOM	2467	CG2	VAL	405	11.874	13.168	32.805	1.00	21.94
ATOM	2468	C	VAL	405	12.301	15.784	30.018	1.00	20.69
ATOM	2469	O	VAL	405	12.977	16.796	30.231	1.00	18.61
ATOM	2470	N	MET	406	11.324	15.753	29.115	1.00	20.17
ATOM	2471	CA	MET	406	10.981	16.958	28.365	1.00	22.23
ATOM	2472	CB	MET	406	9.872	16.667	27.340	1.00	23.65
ATOM	2473	CG	MET	406	9.561	17.832	26.386	1.00	27.90
ATOM	2474	SD	MET	406	11.012	18.547	25.544	1.00	28.93
ATOM	2475	CE	MET	406	11.188	20.096	26.426	1.00	30.21
ATOM	2476	C	MET	406	10.510	17.921	29.450	1.00	21.91
ATOM	2477	O	MET	406	9.648	17.578	30.255	1.00	21.56
ATOM	2478	N	ASP	407	11.090	19.118	29.479	1.00	21.92
ATOM	2479	CA	ASP	407	10.772	20.088	30.518	1.00	21.23
ATOM	2480	CB	ASP	407	12.080	20.667	31.076	1.00	22.53
ATOM	2481	CG	ASP	407	12.935	21.333	30.010	1.00	22.91
ATOM	2482	OD1	ASP	407	12.698	21.104	28.805	1.00	21.72
ATOM	2483	OD2	ASP	407	13.865	22.080	30.381	1.00	25.05
ATOM	2484	C	ASP	407	9.807	21.231	30.218	1.00	20.11
ATOM	2485	O	ASP	407	9.526	22.033	31.110	1.00	20.70
ATOM	2486	N	ASP	408	9.290	21.323	28.995	1.00	17.35
ATOM	2487	CA	ASP	408	8.360	22.411	28.685	1.00	16.87
ATOM	2488	CB	ASP	408	8.245	22.609	27.161	1.00	17.11
ATOM	2489	CG	ASP	408	7.546	21.452	26.456	1.00	19.43
ATOM	2490	OD1	ASP	408	7.796	20.282	26.819	1.00	22.30
ATOM	2491	OD2	ASP	408	6.760	21.713	25.517	1.00	18.07
ATOM	2492	C	ASP	408	6.999	22.097	29.300	1.00	16.68
ATOM	2493	O	ASP	408	6.758	20.961	29.720	1.00	15.83
ATOM	2494	N	LEU	409	6.127	23.101	29.387	1.00	13.90
ATOM	2495	CA	LEU	409	4.794	22.909	29.956	1.00	13.76
ATOM	2496	CB	LEU	409	4.736	23.487	31.374	1.00	13.53
ATOM	2497	CG	LEU	409	5.650	22.862	32.430	1.00	14.07
ATOM	2498	CD1	LEU	409	6.762	23.836	32.784	1.00	12.29
ATOM	2499	CD2	LEU	409	4.839	22.509	33.663	1.00	12.48
ATOM	2500	C	LEU	409	3.686	23.555	29.116	1.00	14.21
ATOM	2501	O	LEU	409	3.852	24.668	28.612	1.00	16.23
ATOM	2502	N	LYS	410	2.552	22.867	28.969	1.00	12.65
ATOM	2503	CA	LYS	410	1.430	23.420	28.208	1.00	10.78
ATOM	2504	CB	LYS	410	1.008	22.466	27.084	1.00	11.42
ATOM	2505	CG	LYS	410	2.100	22.181	26.045	1.00	10.36

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ATOM   2506  CD  LYS   410       2.470  23.418  25.242  1.00 11.81
ATOM   2507  CE  LYS   410       3.346  23.053  24.046  1.00 13.76
ATOM   2508  NZ  LYS   410       3.661  24.235  23.178  1.00 17.24
ATOM   2509  C   LYS   410       0.268  23.661  29.171  1.00  9.91
ATOM   2510  O   LYS   410      -0.254  22.725  29.781  1.00  9.92
ATOM   2511  N   SER   411      -0.142  24.920  29.299  1.00  8.88
ATOM   2512  CA  SER   411      -1.205  25.290  30.228  1.00  9.10
ATOM   2513  CB  SER   411      -2.563  24.754  29.762  1.00  8.30
ATOM   2514  OG  SER   411      -3.030  25.489  28.638  1.00  9.25
ATOM   2515  C   SER   411      -0.879  24.773  31.629  1.00  9.89
ATOM   2516  O   SER   411      -1.770  24.381  32.389  1.00  8.39
ATOM   2517  N   GLY   412       0.412  24.770  31.958  1.00  8.24
ATOM   2518  CA  GLY   412       0.845  24.329  33.276  1.00 10.41
ATOM   2519  C   GLY   412       1.058  22.833  33.458  1.00 11.94
ATOM   2520  O   GLY   412       1.555  22.407  34.495  1.00 12.76
ATOM   2521  N   VAL   413       0.694  22.039  32.454  1.00 10.90
ATOM   2522  CA  VAL   413       0.830  20.581  32.525  1.00 11.21
ATOM   2523  CB  VAL   413      -0.340  19.881  31.791  1.00 10.15
ATOM   2524  CG1 VAL   413      -0.230  18.349  31.945  1.00  7.77
ATOM   2525  CG2 VAL   413      -1.667  20.395  32.330  1.00  7.83
ATOM   2526  C   VAL   413       2.125  20.055  31.914  1.00 11.70
ATOM   2527  O   VAL   413       2.440  20.349  30.757  1.00 13.29
ATOM   2528  N   PRO   414       2.898  19.270  32.681  1.00 12.85
ATOM   2529  CD  PRO   414       2.814  19.068  34.140  1.00 12.82
ATOM   2530  CA  PRO   414       4.153  18.722  32.153  1.00 13.48
ATOM   2531  CB  PRO   414       4.906  18.306  33.415  1.00 13.60
ATOM   2532  CG  PRO   414       3.803  17.956  34.365  1.00 14.61
ATOM   2533  C   PRO   414       3.936  17.549  31.193  1.00 13.05
ATOM   2534  O   PRO   414       2.876  16.915  31.188  1.00 12.46
ATOM   2535  N   ARG   415       4.950  17.278  30.381  1.00 12.89
ATOM   2536  CA  ARG   415       4.921  16.197  29.406  1.00 12.39
ATOM   2537  CB  ARG   415       6.269  16.136  28.685  1.00 14.39
ATOM   2538  CG  ARG   415       6.550  17.332  27.808  1.00 13.44
ATOM   2539  CD  ARG   415       6.004  17.118  26.407  1.00 14.29
ATOM   2540  NE  ARG   415       6.064  18.339  25.613  1.00 14.30
ATOM   2541  CZ  ARG   415       5.610  18.445  24.368  1.00 15.85
ATOM   2542  NH1 ARG   415       5.063  17.392  23.767  1.00 14.69
ATOM   2543  NH2 ARG   415       5.693  19.606  23.731  1.00 14.92
ATOM   2544  C   ARG   415       4.644  14.859  30.082  1.00 10.19
ATOM   2545  O   ARG   415       5.385  14.453  30.977  1.00  8.07
ATOM   2546  N   ALA   416       3.580  14.187  29.646  1.00 10.58
ATOM   2547  CA  ALA   416       3.166  12.888  30.187  1.00  8.73
ATOM   2548  CB  ALA   416       4.272  11.843  29.965  1.00  9.75
ATOM   2549  C   ALA   416       2.794  12.947  31.670  1.00 11.26
ATOM   2550  O   ALA   416       2.716  11.917  32.346  1.00 11.66
ATOM   2551  N   GLY   417       2.549  14.148  32.175  1.00  9.96
ATOM   2552  CA  GLY   417       2.200  14.284  33.579  1.00 10.66
ATOM   2553  C   GLY   417       0.772  13.907  33.919  1.00 10.61
ATOM   2554  O   GLY   417      -0.134  14.016  33.089  1.00  8.74
ATOM   2555  N   TYR   418       0.580  13.442  35.148  1.00 11.30
ATOM   2556  CA  TYR   418      -0.736  13.072  35.658  1.00 11.03
ATOM   2557  CB  TYR   418      -0.956  11.559  35.613  1.00 12.16
ATOM   2558  CG  TYR   418      -2.378  11.192  35.938  1.00 12.39
ATOM   2559  CD1 TYR   418      -3.420  11.574  35.094  1.00 13.22
ATOM   2560  CE1 TYR   418      -4.748  11.278  35.408  1.00 13.88
ATOM   2561  CD2 TYR   418      -2.695  10.504  37.107  1.00 12.99
ATOM   2562  CE2 TYR   418      -4.019  10.204  37.433  1.00 15.09
ATOM   2563  CZ  TYR   418      -5.036  10.594  36.578  1.00 14.68
ATOM   2564  OH  TYR   418      -6.340  10.301  36.884  1.00 13.85
ATOM   2565  C   TYR   418      -0.739  13.546  37.108  1.00 11.47
ATOM   2566  O   TYR   418       0.060  13.077  37.911  1.00 11.42
ATOM   2567  N   ARG   419      -1.645  14.468  37.435  1.00 11.84
ATOM   2568  CA  ARG   419      -1.711  15.056  38.769  1.00 10.81
ATOM   2569  CB  ARG   419      -2.153  14.029  39.816  1.00 12.73
ATOM   2570  CG  ARG   419      -3.565  13.484  39.577  1.00 14.51
ATOM   2571  CD  ARG   419      -4.089  12.741  40.795  1.00 16.79
ATOM   2572  NE  ARG   419      -4.248  13.631  41.945  1.00 17.77
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ATOM	2573	CZ	ARG	419	-5.258	14.485	42.099	1.00	18.81
ATOM	2574	NH1	ARG	419	-6.211	14.565	41.178	1.00	16.45
ATOM	2575	NH2	ARG	419	-5.314	15.266	43.173	1.00	18.51
ATOM	2576	C	ARG	419	-0.317	15.592	39.082	1.00	12.32
ATOM	2577	O	ARG	419	0.156	15.538	40.225	1.00	12.24
ATOM	2578	N	GLY	420	0.334	16.089	38.030	1.00	9.66
ATOM	2579	CA	GLY	420	1.666	16.672	38.128	1.00	11.13
ATOM	2580	C	GLY	420	2.819	15.680	38.111	1.00	10.62
ATOM	2581	O	GLY	420	3.981	16.063	38.017	1.00	12.09
ATOM	2582	N	ILE	421	2.490	14.400	38.180	1.00	10.95
ATOM	2583	CA	ILE	421	3.496	13.345	38.218	1.00	9.84
ATOM	2584	CB	ILE	421	2.937	12.118	38.966	1.00	11.38
ATOM	2585	CG2	ILE	421	4.007	11.046	39.102	1.00	8.42
ATOM	2586	CG1	ILE	421	2.408	12.548	40.334	1.00	9.50
ATOM	2587	CD1	ILE	421	1.388	11.590	40.916	1.00	8.88
ATOM	2588	C	ILE	421	3.992	12.877	36.859	1.00	10.64
ATOM	2589	O	ILE	421	3.202	12.450	36.013	1.00	8.27
ATOM	2590	N	VAL	422	5.305	12.960	36.655	1.00	10.27
ATOM	2591	CA	VAL	422	5.923	12.499	35.418	1.00	10.24
ATOM	2592	CB	VAL	422	6.933	13.526	34.860	1.00	8.78
ATOM	2593	CG1	VAL	422	7.556	13.000	33.559	1.00	8.47
ATOM	2594	CG2	VAL	422	6.224	14.842	34.597	1.00	5.57
ATOM	2595	C	VAL	422	6.645	11.199	35.781	1.00	11.50
ATOM	2596	O	VAL	422	7.549	11.189	36.633	1.00	12.02
ATOM	2597	N	THR	423	6.227	10.104	35.146	1.00	12.85
ATOM	2598	CA	THR	423	6.797	8.777	35.410	1.00	11.08
ATOM	2599	CB	THR	423	5.670	7.754	35.699	1.00	11.97
ATOM	2600	OG1	THR	423	4.971	8.155	36.884	1.00	12.52
ATOM	2601	CG2	THR	423	6.236	6.348	35.899	1.00	12.25
ATOM	2602	C	THR	423	7.641	8.299	34.235	1.00	12.25
ATOM	2603	O	THR	423	7.220	8.387	33.081	1.00	10.60
ATOM	2604	N	PHE	424	8.831	7.793	34.538	1.00	8.92
ATOM	2605	CA	PHE	424	9.754	7.342	33.505	1.00	10.61
ATOM	2606	CB	PHE	424	10.441	8.569	32.888	1.00	12.21
ATOM	2607	CG	PHE	424	11.135	9.454	33.903	1.00	12.43
ATOM	2608	CD1	PHE	424	12.512	9.362	34.112	1.00	12.34
ATOM	2609	CD2	PHE	424	10.406	10.372	34.656	1.00	12.83
ATOM	2610	CE1	PHE	424	13.154	10.183	35.065	1.00	9.62
ATOM	2611	CE2	PHE	424	11.038	11.191	35.607	1.00	12.28
ATOM	2612	CZ	PHE	424	12.416	11.090	35.807	1.00	12.24
ATOM	2613	C	PHE	424	10.802	6.418	34.097	1.00	9.21
ATOM	2614	O	PHE	424	10.830	6.199	35.311	1.00	8.63
ATOM	2615	N	LEU	425	11.656	5.867	33.240	1.00	10.44
ATOM	2616	CA	LEU	425	12.739	5.005	33.705	1.00	12.86
ATOM	2617	CB	LEU	425	12.844	3.729	32.856	1.00	13.44
ATOM	2618	CG	LEU	425	13.390	2.496	33.591	1.00	15.80
ATOM	2619	CD1	LEU	425	12.397	2.066	34.662	1.00	13.66
ATOM	2620	CD2	LEU	425	13.627	1.356	32.620	1.00	14.67
ATOM	2621	C	LEU	425	14.028	5.820	33.582	1.00	12.64
ATOM	2622	O	LEU	425	14.216	6.564	32.610	1.00	13.34
ATOM	2623	N	PHE	426	14.895	5.711	34.581	1.00	13.75
ATOM	2624	CA	PHE	426	16.166	6.427	34.564	1.00	14.08
ATOM	2625	CB	PHE	426	16.137	7.646	35.489	1.00	16.03
ATOM	2626	CG	PHE	426	17.321	8.557	35.316	1.00	15.63
ATOM	2627	CD1	PHE	426	17.363	9.476	34.270	1.00	17.38
ATOM	2628	CD2	PHE	426	18.414	8.468	36.175	1.00	18.07
ATOM	2629	CE1	PHE	426	18.477	10.296	34.081	1.00	18.16
ATOM	2630	CE2	PHE	426	19.533	9.279	35.995	1.00	19.19
ATOM	2631	CZ	PHE	426	19.568	10.196	34.948	1.00	19.01
ATOM	2632	C	PHE	426	17.245	5.468	35.037	1.00	15.16
ATOM	2633	O	PHE	426	17.266	5.065	36.203	1.00	15.37
ATOM	2634	N	ARG	427	18.134	5.105	34.121	1.00	14.82
ATOM	2635	CA	ARG	427	19.218	4.187	34.413	1.00	15.17
ATOM	2636	CB	ARG	427	20.287	4.896	35.249	1.00	16.57
ATOM	2637	CG	ARG	427	20.768	6.181	34.590	1.00	17.43
ATOM	2638	CD	ARG	427	21.973	6.795	35.281	1.00	19.63
ATOM	2639	NE	ARG	427	23.182	5.990	35.123	1.00	21.31

ATOM	2640	CZ	ARG	427	24.383	6.378	35.539	1.00	21.06
ATOM	2641	NH1	ARG	427	24.521	7.553	36.131	1.00	20.50
ATOM	2642	NH2	ARG	427	25.442	5.598	35.364	1.00	20.79
ATOM	2643	C	ARG	427	18.708	2.935	35.119	1.00	14.88
ATOM	2644	O	ARG	427	19.264	2.505	36.124	1.00	14.49
ATOM	2645	N	GLY	428	17.629	2.368	34.582	1.00	14.59
ATOM	2646	CA	GLY	428	17.048	1.156	35.133	1.00	14.18
ATOM	2647	C	GLY	428	16.131	1.327	36.331	1.00	13.42
ATOM	2648	O	GLY	428	15.552	0.358	36.823	1.00	13.64
ATOM	2649	N	ARG	429	15.979	2.557	36.800	1.00	13.50
ATOM	2650	CA	ARG	429	15.133	2.803	37.957	1.00	12.34
ATOM	2651	CB	ARG	429	15.913	3.607	39.004	1.00	14.51
ATOM	2652	CG	ARG	429	15.047	4.215	40.091	1.00	15.10
ATOM	2653	CD	ARG	429	15.834	4.513	41.350	1.00	17.95
ATOM	2654	NE	ARG	429	17.140	5.144	41.133	1.00	17.71
ATOM	2655	CZ	ARG	429	18.115	5.116	42.040	1.00	17.23
ATOM	2656	NH1	ARG	429	17.914	4.497	43.194	1.00	16.69
ATOM	2657	NH2	ARG	429	19.288	5.687	41.801	1.00	17.62
ATOM	2658	C	ARG	429	13.832	3.512	37.610	1.00	10.16
ATOM	2659	O	ARG	429	13.811	4.439	36.797	1.00	9.63
ATOM	2660	N	ARG	430	12.741	3.059	38.216	1.00	9.43
ATOM	2661	CA	ARG	430	11.444	3.683	37.986	1.00	10.57
ATOM	2662	CB	ARG	430	10.305	2.766	38.441	1.00	11.15
ATOM	2663	CG	ARG	430	8.933	3.414	38.342	1.00	10.88
ATOM	2664	CD	ARG	430	8.655	3.897	36.918	1.00	9.84
ATOM	2665	NE	ARG	430	8.579	2.782	35.982	1.00	8.78
ATOM	2666	CZ	ARG	430	8.575	2.909	34.660	1.00	9.60
ATOM	2667	NH1	ARG	430	8.642	4.117	34.105	1.00	9.70
ATOM	2668	NH2	ARG	430	8.524	1.821	33.891	1.00	7.30
ATOM	2669	C	ARG	430	11.430	4.969	38.796	1.00	11.06
ATOM	2670	O	ARG	430	11.646	4.953	40.018	1.00	12.27
ATOM	2671	N	VAL	431	11.188	6.083	38.121	1.00	8.52
ATOM	2672	CA	VAL	431	11.177	7.370	38.799	1.00	9.78
ATOM	2673	CB	VAL	431	12.360	8.245	38.329	1.00	9.68
ATOM	2674	CG1	VAL	431	12.307	9.612	38.991	1.00	9.86
ATOM	2675	CG2	VAL	431	13.678	7.545	38.655	1.00	9.92
ATOM	2676	C	VAL	431	9.895	8.146	38.576	1.00	10.38
ATOM	2677	O	VAL	431	9.370	8.199	37.455	1.00	8.66
ATOM	2678	N	HIS	432	9.395	8.736	39.657	1.00	9.22
ATOM	2679	CA	HIS	432	8.202	9.568	39.610	1.00	9.89
ATOM	2680	CB	HIS	432	7.130	9.066	40.585	1.00	9.64
ATOM	2681	CG	HIS	432	6.691	7.661	40.335	1.00	11.65
ATOM	2682	CD2	HIS	432	6.876	6.528	41.056	1.00	10.40
ATOM	2683	ND1	HIS	432	5.999	7.287	39.204	1.00	11.22
ATOM	2684	CE1	HIS	432	5.777	5.985	39.238	1.00	11.00
ATOM	2685	NE2	HIS	432	6.299	5.500	40.350	1.00	11.59
ATOM	2686	C	HIS	432	8.591	10.990	40.020	1.00	10.06
ATOM	2687	O	HIS	432	8.712	11.281	41.212	1.00	12.29
ATOM	2688	N	LEU	433	8.822	11.865	39.045	1.00	10.25
ATOM	2689	CA	LEU	433	9.131	13.258	39.351	1.00	12.38
ATOM	2690	CB	LEU	433	9.620	14.003	38.099	1.00	11.80
ATOM	2691	CG	LEU	433	9.990	15.488	38.245	1.00	11.29
ATOM	2692	CD1	LEU	433	11.205	15.640	39.160	1.00	13.12
ATOM	2693	CD2	LEU	433	10.297	16.083	36.871	1.00	13.34
ATOM	2694	C	LEU	433	7.745	13.746	39.757	1.00	12.80
ATOM	2695	O	LEU	433	6.864	13.888	38.905	1.00	9.26
ATOM	2696	N	ALA	434	7.544	13.988	41.052	1.00	12.83
ATOM	2697	CA	ALA	434	6.226	14.393	41.532	1.00	12.36
ATOM	2698	CB	ALA	434	5.557	13.207	42.228	1.00	11.99
ATOM	2699	C	ALA	434	6.183	15.596	42.455	1.00	12.54
ATOM	2700	O	ALA	434	7.171	15.939	43.108	1.00	10.67
ATOM	2701	N	PRO	435	5.017	16.255	42.524	1.00	14.34
ATOM	2702	CD	PRO	435	3.802	16.051	41.707	1.00	12.90
ATOM	2703	CA	PRO	435	4.867	17.423	43.392	1.00	14.91
ATOM	2704	CB	PRO	435	3.719	18.180	42.739	1.00	15.50
ATOM	2705	CG	PRO	435	2.814	17.047	42.322	1.00	14.09
ATOM	2706	C	PRO	435	4.479	16.886	44.761	1.00	16.21

ATOM	2707	O	PRO	435	4.265	15.677	44.913	1.00	14.60
ATOM	2708	N	PRO	436	4.382	17.767	45.774	1.00	16.50
ATOM	2709	CD	PRO	436	4.698	19.205	45.790	1.00	16.85
ATOM	2710	CA	PRO	436	4.001	17.303	47.112	1.00	16.19
ATOM	2711	CB	PRO	436	4.026	18.580	47.947	1.00	16.46
ATOM	2712	CG	PRO	436	5.038	19.433	47.247	1.00	17.21
ATOM	2713	C	PRO	436	2.597	16.719	47.020	1.00	17.81
ATOM	2714	O	PRO	436	1.814	17.110	46.153	1.00	15.08
ATOM	2715	N	GLN	437	2.283	15.793	47.918	1.00	18.33
ATOM	2716	CA	GLN	437	0.984	15.129	47.938	1.00	20.68
ATOM	2717	CB	GLN	437	0.998	14.047	49.024	1.00	21.78
ATOM	2718	CG	GLN	437	-0.273	13.238	49.150	1.00	24.75
ATOM	2719	CD	GLN	437	-0.014	11.871	49.753	1.00	25.93
ATOM	2720	OE1	GLN	437	0.814	11.728	50.657	1.00	28.65
ATOM	2721	NE2	GLN	437	-0.723	10.859	49.259	1.00	22.55
ATOM	2722	C	GLN	437	-0.195	16.080	48.142	1.00	20.15
ATOM	2723	O	GLN	437	-1.358	15.675	48.068	1.00	20.67
ATOM	2724	N	THR	438	0.107	17.347	48.389	1.00	20.34
ATOM	2725	CA	THR	438	-0.930	18.345	48.591	1.00	20.14
ATOM	2726	CB	THR	438	-0.447	19.442	49.548	1.00	21.75
ATOM	2727	OG1	THR	438	0.793	19.972	49.072	1.00	20.60
ATOM	2728	CG2	THR	438	-0.251	18.874	50.953	1.00	22.20
ATOM	2729	C	THR	438	-1.353	18.983	47.266	1.00	20.87
ATOM	2730	O	THR	438	-2.198	19.884	47.242	1.00	18.99
ATOM	2731	N	TRP	439	-0.759	18.513	46.170	1.00	19.51
ATOM	2732	CA	TRP	439	-1.075	19.012	44.832	1.00	18.37
ATOM	2733	CB	TRP	439	-0.542	18.052	43.770	1.00	18.42
ATOM	2734	CG	TRP	439	-0.723	18.524	42.355	1.00	18.26
ATOM	2735	CD2	TRP	439	-1.809	18.208	41.474	1.00	18.69
ATOM	2736	CE2	TRP	439	-1.550	18.852	40.241	1.00	18.52
ATOM	2737	CE3	TRP	439	-2.975	17.442	41.604	1.00	19.01
ATOM	2738	CD1	TRP	439	0.124	19.327	41.644	1.00	19.24
ATOM	2739	NE1	TRP	439	-0.364	19.527	40.372	1.00	18.78
ATOM	2740	CZ2	TRP	439	-2.416	18.753	39.143	1.00	17.66
ATOM	2741	CZ3	TRP	439	-3.838	17.343	40.512	1.00	19.78
ATOM	2742	CH2	TRP	439	-3.551	17.997	39.297	1.00	18.78
ATOM	2743	C	TRP	439	-2.588	19.089	44.702	1.00	18.40
ATOM	2744	O	TRP	439	-3.298	18.180	45.129	1.00	19.46
ATOM	2745	N	ASP	440	-3.079	20.158	44.091	1.00	19.35
ATOM	2746	CA	ASP	440	-4.511	20.334	43.931	1.00	21.05
ATOM	2747	CB	ASP	440	-5.072	21.086	45.136	1.00	23.33
ATOM	2748	CG	ASP	440	-6.579	20.992	45.229	1.00	27.35
ATOM	2749	OD1	ASP	440	-7.172	21.753	46.022	1.00	29.50
ATOM	2750	OD2	ASP	440	-7.171	20.147	44.517	1.00	29.29
ATOM	2751	C	ASP	440	-4.873	21.094	42.656	1.00	20.72
ATOM	2752	O	ASP	440	-5.579	22.104	42.710	1.00	21.20
ATOM	2753	N	GLY	441	-4.389	20.622	41.513	1.00	17.73
ATOM	2754	CA	GLY	441	-4.709	21.293	40.264	1.00	16.49
ATOM	2755	C	GLY	441	-3.537	22.011	39.623	1.00	16.83
ATOM	2756	O	GLY	441	-2.623	22.481	40.303	1.00	16.95
ATOM	2757	N	TYR	442	-3.573	22.109	38.299	1.00	16.13
ATOM	2758	CA	TYR	442	-2.508	22.753	37.551	1.00	14.86
ATOM	2759	CB	TYR	442	-2.533	22.276	36.099	1.00	13.44
ATOM	2760	CG	TYR	442	-2.189	20.817	35.945	1.00	11.58
ATOM	2761	CD1	TYR	442	-3.182	19.863	35.715	1.00	10.86
ATOM	2762	CE1	TYR	442	-2.858	18.509	35.577	1.00	11.73
ATOM	2763	CD2	TYR	442	-0.864	20.387	36.037	1.00	10.29
ATOM	2764	CE2	TYR	442	-0.533	19.047	35.903	1.00	9.50
ATOM	2765	CZ	TYR	442	-1.531	18.111	35.675	1.00	10.92
ATOM	2766	OH	TYR	442	-1.201	16.777	35.569	1.00	9.57
ATOM	2767	C	TYR	442	-2.556	24.275	37.583	1.00	15.63
ATOM	2768	O	TYR	442	-3.604	24.877	37.821	1.00	17.47
ATOM	2769	N	ASP	443	-1.406	24.888	37.329	1.00	14.90
ATOM	2770	CA	ASP	443	-1.284	26.343	37.306	1.00	15.25
ATOM	2771	CB	ASP	443	-0.301	26.798	38.385	1.00	15.77
ATOM	2772	CG	ASP	443	-0.282	28.301	38.559	1.00	16.98
ATOM	2773	OD1	ASP	443	-0.755	29.007	37.646	1.00	18.44

ATOM	2774	OD2	ASP	443	0.212	28.778	39.603	1.00	20.07
ATOM	2775	C	ASP	443	-0.763	26.741	35.930	1.00	14.83
ATOM	2776	O	ASP	443	0.411	26.539	35.625	1.00	17.67
ATOM	2777	N	PRO	444	-1.628	27.309	35.076	1.00	14.92
ATOM	2778	CD	PRO	444	-3.052	27.632	35.284	1.00	15.88
ATOM	2779	CA	PRO	444	-1.187	27.707	33.734	1.00	14.37
ATOM	2780	CB	PRO	444	-2.481	28.191	33.075	1.00	16.00
ATOM	2781	CG	PRO	444	-3.292	28.694	34.239	1.00	17.69
ATOM	2782	C	PRO	444	-0.070	28.745	33.711	1.00	13.38
ATOM	2783	O	PRO	444	0.572	28.949	32.678	1.00	14.27
ATOM	2784	N	SER	445	0.184	29.382	34.850	1.00	13.17
ATOM	2785	CA	SER	445	1.241	30.387	34.923	1.00	14.27
ATOM	2786	CB	SER	445	1.070	31.282	36.165	1.00	15.58
ATOM	2787	OG	SER	445	1.196	30.553	37.372	1.00	14.66
ATOM	2788	C	SER	445	2.615	29.724	34.932	1.00	15.28
ATOM	2789	O	SER	445	3.640	30.402	34.822	1.00	15.96
ATOM	2790	N	TRP	446	2.634	28.399	35.075	1.00	15.77
ATOM	2791	CA	TRP	446	3.890	27.647	35.050	1.00	16.19
ATOM	2792	CB	TRP	446	3.717	26.254	35.676	1.00	15.38
ATOM	2793	CG	TRP	446	3.830	26.193	37.194	1.00	15.93
ATOM	2794	CD2	TRP	446	4.527	25.198	37.968	1.00	14.95
ATOM	2795	CE2	TRP	446	4.320	25.505	39.333	1.00	16.05
ATOM	2796	CE3	TRP	446	5.305	24.079	37.638	1.00	13.18
ATOM	2797	CD1	TRP	446	3.247	27.038	38.102	1.00	18.25
ATOM	2798	NE1	TRP	446	3.538	26.630	39.388	1.00	17.18
ATOM	2799	CZ2	TRP	446	4.864	24.730	40.369	1.00	16.85
ATOM	2800	CZ3	TRP	446	5.846	23.309	38.668	1.00	14.20
ATOM	2801	CH2	TRP	446	5.621	23.640	40.017	1.00	14.63
ATOM	2802	C	TRP	446	4.186	27.511	33.565	1.00	15.71
ATOM	2803	O	TRP	446	3.523	26.747	32.869	1.00	15.59
ATOM	2804	N	THR	447	5.162	28.268	33.074	1.00	16.67
ATOM	2805	CA	THR	447	5.507	28.227	31.658	1.00	17.48
ATOM	2806	CB	THR	447	5.180	29.568	30.962	1.00	16.16
ATOM	2807	OG1	THR	447	5.920	30.626	31.586	1.00	19.66
ATOM	2808	CG2	THR	447	3.685	29.879	31.071	1.00	17.91
ATOM	2809	C	THR	447	6.976	27.908	31.424	1.00	17.63
ATOM	2810	O	THR	447	7.714	27.735	32.412	1.00	16.64
ATOM	2811	OT2	THR	447	7.369	27.837	30.242	1.00	20.63
ATOM	2812	MN+2	MN2	448	5.270	16.183	11.594	1.00	13.55
ATOM	2813	C1'	UD1	449	2.930	19.714	14.651	1.00	30.36
ATOM	2814	C2'	UD1	449	2.466	18.449	15.385	1.00	31.86
ATOM	2815	C3'	UD1	449	1.186	17.965	14.683	1.00	29.74
ATOM	2816	C4'	UD1	449	0.045	18.995	14.752	1.00	27.62
ATOM	2817	C5'	UD1	449	0.561	20.441	14.385	1.00	27.14
ATOM	2818	C6'	UD1	449	-0.356	21.505	14.985	1.00	25.41
ATOM	2819	C7'	UD1	449	3.992	16.964	16.558	1.00	36.77
ATOM	2820	C8'	UD1	449	5.048	15.929	16.456	1.00	36.23
ATOM	2821	N2'	UD1	449	3.493	17.380	15.401	1.00	34.92
ATOM	2822	O1'	UD1	449	3.036	19.406	13.237	1.00	29.30
ATOM	2823	O3'	UD1	449	0.817	16.720	15.297	1.00	33.06
ATOM	2824	O4'	UD1	449	-0.939	18.650	13.768	1.00	23.02
ATOM	2825	O5'	UD1	449	1.933	20.726	14.834	1.00	30.30
ATOM	2826	O6'	UD1	449	-0.164	22.723	14.277	1.00	22.40
ATOM	2827	O7'	UD1	449	3.603	17.342	17.676	1.00	35.08
ATOM	2828	N1	UD1	449	-0.691	19.424	6.888	1.00	13.74
ATOM	2829	C2	UD1	449	-1.883	19.843	6.305	1.00	13.35
ATOM	2830	N3	UD1	449	-1.856	20.973	5.588	1.00	12.33
ATOM	2831	C4	UD1	449	-0.794	21.772	5.397	1.00	13.97
ATOM	2832	C5	UD1	449	0.497	21.387	6.003	1.00	15.23
ATOM	2833	C6	UD1	449	0.553	20.238	6.720	1.00	14.05
ATOM	2834	O2	UD1	449	-2.963	19.262	6.393	1.00	14.42
ATOM	2835	O4	UD1	449	-0.866	22.725	4.633	1.00	13.05
ATOM	2836	C1*	UD1	449	-0.667	18.177	7.679	1.00	15.12
ATOM	2837	C2*	UD1	449	0.479	17.191	7.346	1.00	13.41
ATOM	2838	O2*	UD1	449	0.124	16.442	6.171	1.00	14.56
ATOM	2839	C3*	UD1	449	0.595	16.379	8.659	1.00	14.48
ATOM	2840	C4*	UD1	449	0.126	17.405	9.728	1.00	15.16

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ATOM   2841  O4*  UD1     449      -0.548  18.464   9.051  1.00 13.62
ATOM   2842  O3*  UD1     449      -0.357  15.308   8.619  1.00 16.89
ATOM   2843  C5*  UD1     449       1.308  18.093  10.486  1.00 15.99
ATOM   2844  O5*  UD1     449       2.286  18.720   9.632  1.00 15.64
ATOM   2845  PA   UD1     449       3.828  18.574   9.836  1.00 18.78
ATOM   2846  O1A  UD1     449       4.411  19.019   8.536  1.00 15.07
ATOM   2847  O2A  UD1     449       4.158  17.180  10.097  1.00 16.76
ATOM   2848  O3A  UD1     449       4.211  19.467  10.979  1.00 19.54
ATOM   2849  PB   UD1     449       4.444  19.229  12.517  1.00 25.57
ATOM   2850  O1B  UD1     449       5.448  20.167  13.068  1.00 28.22
ATOM   2851  O2B  UD1     449       4.784  17.802  12.779  1.00 21.74
ATOM   2852  C1   GOL A  450     -10.579  -0.719   2.324  1.00 18.35      A
ATOM   2853  O1   GOL A  450      -9.954  -1.827   2.939  1.00 17.02      A
ATOM   2854  C2   GOL A  450     -10.633   0.471   3.276  1.00 19.67      A
ATOM   2855  O2   GOL A  450      -9.314   0.729   3.775  1.00 18.64      A
ATOM   2856  C3   GOL A  450     -11.158   1.709   2.544  1.00 19.85      A
ATOM   2857  O3   GOL A  450     -11.138   2.848   3.383  1.00 21.28      A
ATOM   2858  C1   GOL B  451       1.885  23.415  37.545  1.00 25.04      B
ATOM   2859  O1   GOL B  451       0.585  23.353  36.991  1.00 21.14      B
ATOM   2860  C2   GOL B  451       2.115  22.284  38.550  1.00 26.40      B
ATOM   2861  O2   GOL B  451       1.095  22.327  39.553  1.00 26.92      B
ATOM   2862  C3   GOL B  451       2.070  20.925  37.854  1.00 26.88      B
ATOM   2863  O3   GOL B  451       2.236  19.880  38.793  1.00 29.80      B
ATOM   2864  OH2  TIP S    1      -2.619  14.449  15.319  1.00  6.24      S
ATOM   2865  OH2  TIP S    2      -0.038  14.491  42.729  1.00  8.17      S
ATOM   2866  OH2  TIP S    3      -5.337  21.683  30.864  1.00 12.36      S
ATOM   2867  OH2  TIP S    4      -2.654  23.918  13.946  1.00 11.74      S
ATOM   2868  OH2  TIP S    5       0.328   8.338  35.356  1.00 11.60      S
ATOM   2869  OH2  TIP S    6       2.999  15.307  22.130  1.00 10.24      S
ATOM   2870  OH2  TIP S    7     -13.858  20.819  25.270  1.00 10.44      S
ATOM   2871  OH2  TIP S    8       9.030   7.210  29.930  1.00  9.07      S
ATOM   2872  OH2  TIP S    9      -1.766  -4.335  15.619  1.00  4.66      S
ATOM   2873  OH2  TIP S   10       1.338   9.507  31.866  1.00 11.77      S
ATOM   2874  OH2  TIP S   11       1.719  13.737   2.508  1.00  7.14      S
ATOM   2875  OH2  TIP S   12     -16.839  19.244   1.642  1.00 12.38      S
ATOM   2876  OH2  TIP S   13       3.139  38.470  12.102  1.00  9.09      S
ATOM   2877  OH2  TIP S   14       4.764  35.891  12.908  1.00 10.53      S
ATOM   2878  OH2  TIP S   16       7.481  18.699  30.696  1.00  9.66      S
ATOM   2879  OH2  TIP S   17      -1.662  -3.319  30.331  1.00  8.88      S
ATOM   2880  OH2  TIP S   18       8.681   4.892  23.181  1.00 11.65      S
ATOM   2881  OH2  TIP S   19      -1.893  11.702  14.779  1.00  8.32      S
ATOM   2882  OH2  TIP S   20      -6.008  23.435   4.927  1.00  9.40      S
ATOM   2883  OH2  TIP S   21       9.854  -5.273  24.515  1.00 14.15      S
ATOM   2884  OH2  TIP S   22       7.601  25.477  29.112  1.00 15.00      S
ATOM   2885  OH2  TIP S   23      -6.838  41.838  13.670  1.00 12.83      S
ATOM   2886  OH2  TIP S   24       5.370  11.652   5.322  1.00 10.28      S
ATOM   2887  OH2  TIP S   25      -3.364  18.306  27.994  1.00 11.43      S
ATOM   2888  OH2  TIP S   26       3.562  28.551   8.636  1.00 16.52      S
ATOM   2889  OH2  TIP S   27      -4.446  23.418  32.822  1.00 11.65      S
ATOM   2890  OH2  TIP S   28      -0.505  15.351  17.032  1.00  8.28      S
ATOM   2891  OH2  TIP S   29       8.734  14.219  -8.603  1.00 34.39      S
ATOM   2892  OH2  TIP S   30      -5.055  -0.942  39.880  1.00  9.35      S
ATOM   2893  OH2  TIP S   32      -2.307  20.612  28.919  1.00 15.07      S
ATOM   2894  OH2  TIP S   33       6.565  -0.561  12.026  1.00 18.10      S
ATOM   2895  OH2  TIP S   34     -14.706   9.219  27.153  1.00 10.75      S
ATOM   2896  OH2  TIP S   35      10.074   9.101  17.067  1.00 18.48      S
ATOM   2897  OH2  TIP S   36       7.589  17.745  -4.522  1.00  9.49      S
ATOM   2898  OH2  TIP S   37      18.130  11.493  49.224  1.00 23.39      S
ATOM   2899  OH2  TIP S   39       8.863  -0.837  35.307  1.00 19.46      S
ATOM   2900  OH2  TIP S   40     -19.524  13.748  15.871  1.00  9.00      S
ATOM   2901  OH2  TIP S   41       3.605  14.951  12.790  1.00 13.79      S
ATOM   2902  OH2  TIP S   42      14.737  -1.593  29.630  1.00 17.50      S
ATOM   2903  OH2  TIP S   43       2.467  16.577   4.610  1.00  8.60      S
ATOM   2904  OH2  TIP S   44       2.518   4.041   9.613  1.00 10.14      S
ATOM   2905  OH2  TIP S   45       1.461  35.631  19.162  1.00 11.54      S
ATOM   2906  OH2  TIP S   46       2.388  26.207  30.628  1.00 18.20      S
ATOM   2907  OH2  TIP S   47       2.955   4.386  -6.155  1.00 18.08      S
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ATOM	2908	OH2	TIP	S	48	-9.376	26.330	11.576	1.00	15.54	S
ATOM	2909	OH2	TIP	S	49	16.794	3.119	31.996	1.00	15.71	S
ATOM	2910	OH2	TIP	S	50	-1.664	-7.353	12.845	1.00	15.42	S
ATOM	2911	OH2	TIP	S	51	-6.315	-4.662	35.818	1.00	12.00	S
ATOM	2912	OH2	TIP	S	52	3.743	17.309	-7.641	1.00	13.66	S
ATOM	2913	OH2	TIP	S	53	-4.489	1.417	38.629	1.00	16.55	S
ATOM	2914	OH2	TIP	S	54	0.192	28.521	30.062	1.00	13.21	S
ATOM	2915	OH2	TIP	S	55	5.224	-7.088	35.627	1.00	11.07	S
ATOM	2916	OH2	TIP	S	56	12.959	14.411	46.341	1.00	17.07	S
ATOM	2917	OH2	TIP	S	57	-7.052	13.049	38.673	1.00	21.81	S
ATOM	2918	OH2	TIP	S	59	1.906	-2.724	3.062	1.00	11.07	S
ATOM	2919	OH2	TIP	S	61	-12.970	10.861	22.886	1.00	16.08	S
ATOM	2920	OH2	TIP	S	62	-8.903	30.391	17.233	1.00	14.30	S
ATOM	2921	OH2	TIP	S	63	-5.416	14.819	28.573	1.00	15.28	S
ATOM	2922	OH2	TIP	S	64	15.913	7.066	22.078	1.00	16.08	S
ATOM	2923	OH2	TIP	S	65	-12.031	28.300	21.129	1.00	21.96	S
ATOM	2924	OH2	TIP	S	66	-21.288	19.780	17.280	1.00	17.61	S
ATOM	2925	OH2	TIP	S	67	2.523	9.560	35.763	1.00	11.93	S
ATOM	2926	OH2	TIP	S	71	17.581	6.858	25.586	1.00	24.36	S
ATOM	2927	OH2	TIP	S	72	0.713	32.515	18.931	1.00	14.05	S
ATOM	2928	OH2	TIP	S	73	-10.423	6.702	-3.043	1.00	18.88	S
ATOM	2929	OH2	TIP	S	75	-4.551	27.950	19.772	1.00	17.37	S
ATOM	2930	OH2	TIP	S	76	-9.445	28.117	24.796	1.00	18.43	S
ATOM	2931	OH2	TIP	S	77	4.569	33.150	34.664	1.00	16.60	S
ATOM	2932	OH2	TIP	S	78	1.697	18.165	19.531	1.00	26.10	S
ATOM	2933	OH2	TIP	S	80	6.670	28.083	41.356	1.00	22.43	S
ATOM	2934	OH2	TIP	S	83	-19.032	6.787	19.782	1.00	23.95	S
ATOM	2935	OH2	TIP	S	84	3.508	18.616	5.849	1.00	17.45	S
ATOM	2936	OH2	TIP	S	85	-10.475	-4.104	26.777	1.00	22.60	S
ATOM	2937	OH2	TIP	S	86	-8.648	20.736	32.427	1.00	22.94	S
ATOM	2938	OH2	TIP	S	87	-12.613	13.974	-1.944	1.00	20.59	S
ATOM	2939	OH2	TIP	S	88	5.239	2.923	36.808	1.00	19.57	S
ATOM	2940	OH2	TIP	S	89	6.752	5.980	31.244	1.00	12.28	S
ATOM	2941	OH2	TIP	S	90	-16.084	17.940	6.339	1.00	13.04	S
ATOM	2942	OH2	TIP	S	91	6.948	9.720	30.524	1.00	15.55	S
ATOM	2943	OH2	TIP	S	93	3.418	35.394	17.239	1.00	15.23	S
ATOM	2944	OH2	TIP	S	94	3.978	9.951	33.464	1.00	12.39	S
ATOM	2945	OH2	TIP	S	95	2.754	10.636	26.890	1.00	15.04	S
ATOM	2946	OH2	TIP	S	96	11.032	25.612	42.861	1.00	19.08	S
ATOM	2947	OH2	TIP	S	97	0.160	2.527	35.280	1.00	13.47	S
ATOM	2948	OH2	TIP	S	98	-23.096	8.878	23.466	1.00	23.14	S
ATOM	2949	OH2	TIP	S	100	-3.455	-1.275	-5.511	1.00	28.31	S
ATOM	2950	OH2	TIP	S	102	6.474	15.303	13.450	1.00	15.26	S
ATOM	2951	OH2	TIP	S	105	-1.962	24.741	25.945	1.00	14.19	S
ATOM	2952	OH2	TIP	S	106	-12.616	17.701	-2.912	1.00	21.35	S
ATOM	2953	OH2	TIP	S	107	3.340	31.688	7.182	1.00	23.20	S
ATOM	2954	OH2	TIP	S	108	-7.083	8.885	-5.620	1.00	18.46	S
ATOM	2955	OH2	TIP	S	109	1.200	26.861	27.956	1.00	17.83	S
ATOM	2956	OH2	TIP	S	112	14.452	15.597	25.192	1.00	27.86	S
ATOM	2957	OH2	TIP	S	113	4.417	19.339	21.259	1.00	21.75	S
ATOM	2958	OH2	TIP	S	114	-18.566	22.623	23.139	1.00	27.11	S
ATOM	2959	OH2	TIP	S	115	1.970	42.674	12.973	1.00	18.45	S
ATOM	2960	OH2	TIP	S	117	9.109	-3.025	22.784	1.00	29.39	S
ATOM	2961	OH2	TIP	S	118	-9.411	11.677	37.680	1.00	31.68	S
ATOM	2962	OH2	TIP	S	119	0.951	-7.066	13.578	1.00	20.80	S
ATOM	2963	OH2	TIP	S	122	9.306	4.795	31.263	1.00	20.39	S
ATOM	2964	OH2	TIP	S	123	15.059	18.229	29.238	1.00	20.75	S
ATOM	2965	OH2	TIP	S	124	-12.360	22.961	7.048	1.00	27.64	S
ATOM	2966	OH2	TIP	S	125	-5.725	-5.587	5.346	1.00	27.62	S
ATOM	2967	OH2	TIP	S	126	12.157	3.383	16.976	1.00	24.11	S
ATOM	2968	OH2	TIP	S	128	-8.705	-11.365	22.146	1.00	27.01	S
ATOM	2969	OH2	TIP	S	129	5.152	1.197	-1.254	1.00	21.74	S
ATOM	2970	OH2	TIP	S	132	-7.474	27.681	10.169	1.00	18.55	S
ATOM	2971	OH2	TIP	S	133	-8.144	12.463	34.831	1.00	29.25	S
ATOM	2972	OH2	TIP	S	135	-4.795	24.052	1.761	1.00	14.74	S
ATOM	2973	OH2	TIP	S	137	-7.770	35.250	11.139	1.00	17.78	S
ATOM	2974	OH2	TIP	S	141	2.217	-1.263	0.894	1.00	23.17	S

ATOM	2975	OH2	TIP	S	145	18.073	6.078	31.700	1.00 21.71	S
ATOM	2976	OH2	TIP	S	146	10.774	9.243	51.702	1.00 20.38	S
ATOM	2977	OH2	TIP	S	149	6.383	14.032	46.289	1.00 24.19	S
ATOM	2978	OH2	TIP	S	150	3.993	14.568	49.638	1.00 23.58	S
ATOM	2979	OH2	TIP	S	151	6.935	17.145	10.830	1.00 24.71	S
ATOM	2980	OH2	TIP	S	152	-14.767	11.022	25.127	1.00 16.45	S
ATOM	2981	OH2	TIP	S	155	3.112	34.793	35.963	1.00 13.55	S
ATOM	2982	OH2	TIP	S	156	4.981	20.205	4.172	1.00 22.55	S
ATOM	2983	OH2	TIP	S	157	3.978	0.046	26.997	1.00 16.22	S
ATOM	2984	OH2	TIP	S	158	-9.319	34.584	16.344	1.00 26.08	S
ATOM	2985	OH2	TIP	S	160	19.310	7.919	30.577	1.00 16.97	S
ATOM	2986	OH2	TIP	S	161	10.907	-1.987	21.437	1.00 28.60	S
ATOM	2987	OH2	TIP	S	162	7.153	32.923	35.065	1.00 30.43	S
ATOM	2988	OH2	TIP	S	163	9.779	19.057	11.571	1.00 25.19	S
ATOM	2989	OH2	TIP	S	164	7.653	2.000	3.133	1.00 32.72	S
ATOM	2990	OH2	TIP	S	165	-15.771	12.950	28.240	1.00 21.24	S
ATOM	2991	OH2	TIP	S	166	4.501	22.430	2.978	1.00 22.86	S
ATOM	2992	OH2	TIP	S	167	2.058	19.404	-7.677	1.00 25.69	S
ATOM	2993	OH2	TIP	S	168	-17.529	22.882	25.547	1.00 30.42	S
ATOM	2994	OH2	TIP	S	169	-20.653	9.606	14.310	1.00 18.33	S
ATOM	2995	OH2	TIP	S	170	-6.871	-2.758	39.320	1.00 16.73	S
ATOM	2996	OH2	TIP	S	171	22.388	2.411	50.212	1.00 33.95	S
ATOM	2997	OH2	TIP	S	172	-2.127	27.068	24.420	1.00 34.08	S
ATOM	2998	OH2	TIP	S	174	3.175	33.083	18.156	1.00 26.20	S
ATOM	2999	OH2	TIP	S	176	18.927	16.916	23.138	1.00 32.83	S
ATOM	3000	OH2	TIP	S	177	-2.506	28.076	21.527	1.00 23.81	S
ATOM	3001	OH2	TIP	S	178	3.641	2.269	-7.961	1.00 25.97	S
ATOM	3002	OH2	TIP	S	179	15.097	16.297	45.517	1.00 36.90	S
ATOM	3003	OH2	TIP	S	180	5.712	2.191	46.053	1.00 22.75	S
ATOM	3004	OH2	TIP	S	182	18.991	6.170	39.259	1.00 18.91	S
ATOM	3005	OH2	TIP	S	183	2.030	-8.963	31.389	1.00 21.47	S
ATOM	3006	OH2	TIP	S	184	20.141	4.226	31.090	1.00 26.80	S
ATOM	3007	OH2	TIP	S	185	-12.371	27.358	24.097	1.00 30.84	S
ATOM	3008	OH2	TIP	S	186	-12.410	21.788	-4.264	1.00 21.97	S
ATOM	3009	OH2	TIP	S	187	-13.260	10.420	-2.876	1.00 34.77	S
ATOM	3010	OH2	TIP	S	188	1.626	12.919	27.469	1.00 24.72	S
ATOM	3011	OH2	TIP	S	189	-19.211	1.531	13.688	1.00 27.44	S
ATOM	3012	OH2	TIP	S	190	13.605	7.047	10.423	1.00 33.89	S
ATOM	3013	OH2	TIP	S	191	11.721	-2.092	23.863	1.00 42.27	S
ATOM	3014	OH2	TIP	S	192	6.529	-9.199	18.459	1.00 27.52	S
ATOM	3015	OH2	TIP	S	194	-12.376	0.842	-0.831	1.00 34.72	S
ATOM	3016	OH2	TIP	S	195	6.887	14.513	22.663	1.00 24.22	S
ATOM	3017	OH2	TIP	S	196	-17.161	3.542	34.173	1.00 35.25	S
ATOM	3018	OH2	TIP	S	197	15.301	25.887	37.082	1.00 33.34	S
ATOM	3019	OH2	TIP	S	198	-3.966	12.638	-9.035	1.00 34.32	S
ATOM	3020	OH2	TIP	S	199	-7.343	32.959	17.064	1.00 27.12	S
ATOM	3021	OH2	TIP	S	201	-6.726	-7.569	6.728	1.00 36.08	S
ATOM	3022	OH2	TIP	S	202	-7.611	17.050	44.179	1.00 28.63	S
ATOM	3023	OH2	TIP	S	204	-19.858	5.125	6.110	1.00 28.56	S
ATOM	3024	OH2	TIP	S	205	-11.177	27.534	-3.385	1.00 39.56	S
ATOM	3025	OH2	TIP	S	206	-1.143	6.722	-9.074	1.00 24.68	S
ATOM	3026	OH2	TIP	S	207	17.730	5.447	20.650	1.00 29.57	S
ATOM	3027	OH2	TIP	S	208	-3.142	-1.763	-2.957	1.00 28.13	S
ATOM	3028	OH2	TIP	S	211	-5.045	15.650	-3.992	1.00 23.75	S
ATOM	3029	OH2	TIP	S	212	12.071	1.347	45.877	1.00 25.96	S
ATOM	3030	OH2	TIP	S	213	5.270	21.557	43.008	1.00 25.37	S
ATOM	3031	OH2	TIP	S	214	-10.233	-4.381	29.919	1.00 30.11	S
ATOM	3032	OH2	TIP	S	215	-2.421	14.076	44.280	1.00 27.05	S
ATOM	3033	OH2	TIP	S	216	-19.422	19.722	2.986	1.00 27.27	S
ATOM	3034	OH2	TIP	S	217	20.340	6.622	24.191	1.00 33.05	S
ATOM	3035	OH2	TIP	S	218	-9.287	-10.739	35.371	1.00 23.04	S
ATOM	3036	OH2	TIP	S	220	-18.991	17.956	6.559	1.00 30.74	S
ATOM	3037	OH2	TIP	S	222	-8.230	-1.402	-6.823	1.00 43.42	S
ATOM	3038	OH2	TIP	S	223	4.197	-9.388	24.340	1.00 21.99	S
ATOM	3039	OH2	TIP	S	224	-5.527	24.761	34.893	1.00 31.71	S
ATOM	3040	OH2	TIP	S	226	11.322	8.103	5.203	1.00 31.07	S
ATOM	3041	OH2	TIP	S	227	8.756	16.819	13.810	1.00 31.67	S

ATOM	3042	OH2	TIP	S	228	-7.907	31.804	23.608	1.00	32.60	S
ATOM	3043	OH2	TIP	S	230	-4.851	7.079	46.829	1.00	32.34	S
ATOM	3044	OH2	TIP	S	231	10.341	1.522	7.763	1.00	36.53	S
ATOM	3045	OH2	TIP	S	232	-1.471	22.435	42.612	1.00	20.83	S
ATOM	3046	OH2	TIP	S	233	-8.810	33.613	4.881	1.00	26.21	S
ATOM	3047	OH2	TIP	S	234	-20.756	15.957	16.082	1.00	28.40	S
ATOM	3048	OH2	TIP	S	236	0.865	21.698	46.859	1.00	30.72	S
ATOM	3049	OH2	TIP	S	237	-17.175	-0.197	27.338	1.00	23.66	S
ATOM	3050	OH2	TIP	S	238	-13.091	-1.507	5.188	1.00	39.30	S
ATOM	3051	OH2	TIP	S	239	6.231	-7.875	31.501	1.00	24.11	S
ATOM	3052	OH2	TIP	S	241	-2.273	8.537	-10.616	1.00	29.30	S
ATOM	3053	OH2	TIP	S	242	1.650	13.660	52.902	1.00	36.37	S
ATOM	3054	OH2	TIP	S	244	8.290	-0.218	39.407	1.00	27.91	S
ATOM	3055	OH2	TIP	S	246	-15.816	-1.231	7.398	1.00	27.04	S
ATOM	3056	OH2	TIP	S	249	-6.657	19.034	-1.488	1.00	24.17	S
ATOM	3057	OH2	TIP	S	250	-17.834	15.085	24.642	1.00	26.76	S
ATOM	3058	OH2	TIP	S	253	-5.541	-4.327	2.438	1.00	25.87	S
ATOM	3059	OH2	TIP	S	254	-5.993	4.836	-3.572	1.00	30.43	S
ATOM	3060	OH2	TIP	S	259	7.665	15.134	-4.164	1.00	19.63	S
ATOM	3061	OH2	TIP	S	260	17.850	8.039	16.251	1.00	50.29	S
ATOM	3062	OH2	TIP	S	262	6.950	6.946	51.230	1.00	36.25	S
ATOM	3063	OH2	TIP	S	263	12.332	12.828	27.293	1.00	39.05	S
ATOM	3064	OH2	TIP	S	264	-9.917	4.064	-3.368	1.00	36.12	S
ATOM	3065	OH2	TIP	S	266	-19.316	18.307	15.547	1.00	23.71	S
ATOM	3066	OH2	TIP	S	267	-16.651	12.906	25.780	1.00	20.16	S
ATOM	3067	OH2	TIP	S	270	-2.444	29.149	25.832	1.00	14.00	S
ATOM	3068	OH2	TIP	S	271	18.453	14.389	23.493	1.00	24.67	S
ATOM	3069	OH2	TIP	S	273	19.477	2.189	39.362	1.00	21.88	S
ATOM	3070	OH2	TIP	S	275	4.698	-11.307	20.713	1.00	41.06	S
ATOM	3071	OH2	TIP	S	276	7.614	29.879	34.518	1.00	22.40	S
ATOM	3072	OH2	TIP	S	278	-10.028	29.076	4.799	1.00	20.46	S
ATOM	3073	OH2	TIP	S	279	-9.565	35.766	2.936	1.00	24.75	S
ATOM	3074	OH2	TIP	S	280	-8.295	-5.510	27.151	1.00	28.00	S
ATOM	3075	OH2	TIP	S	281	-11.986	-2.319	29.129	1.00	28.16	S
ATOM	3076	OH2	TIP	S	282	-18.230	17.542	0.448	1.00	44.65	S
ATOM	3077	OH2	TIP	S	283	9.900	33.022	36.410	1.00	32.60	S
ATOM	3078	OH2	TIP	S	284	-20.010	20.865	25.289	1.00	32.70	S
ATOM	3079	OH2	TIP	S	285	-3.185	-3.714	1.057	1.00	29.44	S
ATOM	3080	OH2	TIP	S	286	-15.661	-0.745	36.517	1.00	31.45	S
ATOM	3081	OH2	TIP	S	287	22.717	8.184	50.413	1.00	42.48	S
ATOM	3082	OH2	TIP	S	288	17.538	0.783	40.789	1.00	28.34	S
ATOM	3083	OH2	TIP	S	289	7.379	0.293	-0.546	1.00	38.96	S
ATOM	3084	OH2	TIP	S	290	-9.465	31.278	3.696	1.00	29.29	S
ATOM	3085	OH2	TIP	S	292	14.397	0.534	26.808	1.00	31.83	S
ATOM	3086	OH2	TIP	S	293	-18.844	7.401	26.231	1.00	34.26	S
ATOM	3087	OH2	TIP	S	294	1.507	21.505	44.460	1.00	27.47	S
ATOM	3088	OH2	TIP	S	295	-15.245	28.145	15.662	1.00	24.63	S
ATOM	3089	OH2	TIP	S	296	-3.146	23.568	44.496	1.00	34.23	S
ATOM	3090	OH2	TIP	S	297	28.678	6.073	44.135	1.00	34.39	S
ATOM	3091	OH2	TIP	S	298	-21.657	6.103	14.181	1.00	40.74	S
ATOM	3092	OH2	TIP	S	299	-16.643	27.493	24.298	1.00	41.13	S
ATOM	3093	OH2	TIP	S	300	2.425	21.840	42.100	1.00	28.03	S
ATOM	3094	OH2	TIP	S	301	24.509	5.673	49.231	1.00	50.98	S
ATOM	3095	OH2	TIP	S	302	17.515	18.256	10.204	1.00	35.15	S
ATOM	3096	OH2	TIP	S	303	21.675	0.842	37.222	1.00	33.13	S
ATOM	3097	OH2	TIP	S	304	-17.614	14.043	29.649	1.00	33.21	S
ATOM	3098	OH2	TIP	S	305	-9.860	28.138	7.264	1.00	39.99	S
ATOM	3099	OH2	TIP	S	306	14.253	-1.643	39.289	1.00	39.67	S
ATOM	3100	OH2	TIP	S	307	-6.344	29.635	17.427	1.00	26.70	S
ATOM	3101	OH2	TIP	S	308	3.342	6.949	-7.606	1.00	29.50	S
ATOM	3102	OH2	TIP	S	309	13.305	25.954	44.128	1.00	32.00	S
ATOM	3103	OH2	TIP	S	310	-2.136	24.073	1.657	1.00	49.49	S
ATOM	3104	N	ILE		113	-3.795	11.902	7.822	0.50	7.93	AC2
ATOM	3105	CA	ILE		113	-3.713	13.289	7.378	0.50	7.40	AC2
ATOM	3106	CB	ILE		113	-3.639	14.259	8.582	0.50	6.88	AC2
ATOM	3107	CG2	ILE		113	-3.585	15.705	8.092	0.50	6.81	AC2
ATOM	3108	CG1	ILE		113	-4.856	14.058	9.490	0.50	4.77	AC2

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ATOM   3109  CD1 ILE   113      -6.182  14.283   8.794  0.50  2.46      AC2
ATOM   3110  C   ILE   113      -2.460  13.442   6.524  0.50  8.18      AC2
ATOM   3111  O   ILE   113      -1.352  13.144   6.976  0.50  7.65      AC2
END
```

Table 4

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REMARK Model of GnT I with Acceptor.  GnT I "be" with experimental UDP-
REMARK GlcNAc and Manganese 2+ ion, with Man5GlcNAc2 acceptor modeled into
REMARK the active site.  Ulug Unligil & Dr. James Rini, October 25, 1999.
REMARK coordinates from minimization refinement
REMARK refinement resolution: 50.0 - 1.8 A
REMARK starting r= 0.2113 free_r= 0.2440
REMARK final    r= 0.2103 free_r= 0.2424
REMARK rmsd bonds= 0.005928  rmsd angles=  1.31456
REMARK wa= 1.03895
REMARK target= mlf cycles= 1 steps= 200
REMARK sg= P2(1)2(1)2(1) a= 40.541 b= 82.190 c= 101.956 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:ion.param
REMARK parameter file 3  : ../../../data/udpglcnac.param
REMARK parameter file 4  : CNS_TOPPAR:water_rep.param
REMARK parameter file 5  : CNS_TOPPAR:carbohydrate.param
REMARK molecular structure file: alternate.mtf
REMARK input coordinates: alternate.pdb
REMARK reflection file= ../../../data/gntlbe.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.8
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   4.242 B22=   1.045 B33=  -5.287
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:   -0.095
REMARK bulk solvent: density level= 0.423009 e/A^3, B-factor= 57.5717 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range:     61022 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  18103 (  29.7 % )
REMARK number of reflections rejected:                            0 (   0.0 % )
REMARK total number of reflections used:                      42919 (  70.3 % )
REMARK number of reflections in working set:                  40743 (  66.8 % )
REMARK number of reflections in test set:                      2176 (   3.6 % )
CRYST1   40.541   82.190  101.956  90.00  90.00  90.00 P 21 21 21
REMARK FILENAME="minimize.200.pdb"
REMARK DATE:24-Oct-1999  23:28:47       created by user: ulu
REMARK VERSION:0.9a
ATOM      1  CB  ALA   106     -17.124  -1.055  17.595  1.00 30.32
ATOM      2  C   ALA   106     -16.456  -1.029  15.192  1.00 28.81
ATOM      3  O   ALA   106     -15.342  -1.493  15.418  1.00 29.56
ATOM      4  N   ALA   106     -18.153  -2.641  15.996  1.00 30.51
ATOM      5  CA  ALA   106     -17.606  -1.259  16.162  1.00 29.99
ATOM      6  N   VAL   107     -16.730  -0.309  14.111  1.00 28.51
ATOM      7  CA  VAL   107     -15.706  -0.030  13.115  1.00 26.63
ATOM      8  CB  VAL   107     -16.337   0.167  11.724  1.00 27.28
ATOM      9  CG1 VAL   107     -15.260   0.466  10.703  1.00 26.44
ATOM     10  CG2 VAL   107     -17.110  -1.082  11.329  1.00 27.22
ATOM     11  C   VAL   107     -14.918   1.220  13.496  1.00 25.88
ATOM     12  O   VAL   107     -15.494   2.292  13.686  1.00 26.98
ATOM     13  N   ILE   108     -13.600   1.073  13.602  1.00 22.52
ATOM     14  CA  ILE   108     -12.719   2.180  13.968  1.00 18.62
ATOM     15  CB  ILE   108     -11.829   1.808  15.171  1.00 17.17
ATOM     16  CG2 ILE   108     -10.916   2.981  15.532  1.00 18.17
ATOM     17  CG1 ILE   108     -12.706   1.437  16.369  1.00 17.36
ATOM     18  CD1 ILE   108     -11.919   0.915  17.565  1.00 15.54
ATOM     19  C   ILE   108     -11.819   2.544  12.793  1.00 15.84
ATOM     20  O   ILE   108     -10.843   1.851  12.506  1.00 16.39
ATOM     21  N   PRO   109     -12.138   3.643  12.096  1.00 15.51
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ATOM	22	CD	PRO	109	-13.322	4.508	12.264	1.00	13.90	
ATOM	23	CA	PRO	109	-11.340	4.077	10.949	1.00	13.38	
ATOM	24	CB	PRO	109	-12.283	5.024	10.224	1.00	14.20	
ATOM	25	CG	PRO	109	-12.994	5.683	11.366	1.00	14.48	
ATOM	26	C	PRO	109	-10.040	4.764	11.337	1.00	12.65	
ATOM	27	O	PRO	109	-9.937	5.401	12.396	1.00	9.93	
ATOM	28	N	ILE	110	-9.039	4.603	10.482	1.00	11.19	
ATOM	29	CA	ILE	110	-7.762	5.249	10.698	1.00	9.94	
ATOM	30	CB	ILE	110	-6.570	4.350	10.316	1.00	9.95	
ATOM	31	CG2	ILE	110	-5.259	5.061	10.665	1.00	5.75	
ATOM	32	CG1	ILE	110	-6.671	3.002	11.031	1.00	5.91	
ATOM	33	CD1	ILE	110	-6.678	3.086	12.554	1.00	9.51	
ATOM	34	C	ILE	110	-7.802	6.416	9.729	1.00	10.58	
ATOM	35	O	ILE	110	-7.889	6.215	8.514	1.00	10.62	
ATOM	36	N	LEU	111	-7.772	7.630	10.264	1.00	8.84	
ATOM	37	CA	LEU	111	-7.791	8.818	9.429	1.00	8.46	
ATOM	38	CB	LEU	111	-8.636	9.922	10.070	1.00	9.03	
ATOM	39	CG	LEU	111	-8.517	11.312	9.434	1.00	11.33	
ATOM	40	CD1	LEU	111	-8.911	11.252	7.965	1.00	7.68	
ATOM	41	CD2	LEU	111	-9.403	12.291	10.183	1.00	7.84	
ATOM	42	C	LEU	111	-6.359	9.295	9.270	1.00	9.92	
ATOM	43	O	LEU	111	-5.744	9.765	10.226	1.00	6.35	
ATOM	44	N	VAL	112	-5.827	9.146	8.063	1.00	7.17	
ATOM	45	CA	VAL	112	-4.470	9.577	7.764	1.00	8.54	
ATOM	46	CB	VAL	112	-3.787	8.623	6.751	1.00	11.25	
ATOM	47	CG1	VAL	112	-2.413	9.150	6.369	1.00	10.14	
ATOM	48	CG2	VAL	112	-3.665	7.229	7.351	1.00	5.03	
ATOM	49	C	VAL	112	-4.501	10.985	7.173	1.00	8.75	
ATOM	50	O	VAL	112	-5.162	11.231	6.159	1.00	8.93	
ATOM	51	N	ILE	113	-3.786	11.904	7.813	0.50	8.60	AC1
ATOM	52	CA	ILE	113	-3.717	13.286	7.354	0.50	8.74	AC1
ATOM	53	CB	ILE	113	-3.668	14.279	8.545	0.50	9.65	AC1
ATOM	54	CG2	ILE	113	-3.453	15.701	8.034	0.50	9.68	AC1
ATOM	55	CG1	ILE	113	-4.976	14.217	9.342	0.50	9.12	AC1
ATOM	56	CD1	ILE	113	-5.239	12.886	10.007	0.50	11.25	AC1
ATOM	57	C	ILE	113	-2.460	13.444	6.507	0.50	8.94	AC1
ATOM	58	O	ILE	113	-1.353	13.161	6.967	0.50	8.39	AC1
ATOM	59	N	ALA	114	-2.641	13.887	5.267	1.00	8.94	
ATOM	60	CA	ALA	114	-1.526	14.067	4.340	1.00	10.59	
ATOM	61	CB	ALA	114	-1.535	12.931	3.301	1.00	9.75	
ATOM	62	C	ALA	114	-1.590	15.420	3.638	1.00	10.63	
ATOM	63	O	ALA	114	-2.602	16.114	3.714	1.00	9.04	
ATOM	64	N	CYS	115	-0.510	15.783	2.943	1.00	12.24	
ATOM	65	CA	CYS	115	-0.450	17.065	2.235	1.00	13.22	
ATOM	66	C	CYS	115	0.483	17.061	1.027	1.00	13.96	
ATOM	67	O	CYS	115	0.035	16.900	-0.114	1.00	13.10	
ATOM	68	CB	CYS	115	-0.037	18.167	3.220	1.00	14.16	
ATOM	69	SG	CYS	115	0.498	19.788	2.564	1.00	12.60	
ATOM	70	N	ASP	116	1.780	17.224	1.273	1.00	13.45	
ATOM	71	CA	ASP	116	2.741	17.270	0.182	1.00	13.43	
ATOM	72	CB	ASP	116	3.128	18.729	-0.102	1.00	13.54	
ATOM	73	CG	ASP	116	3.695	19.440	1.118	1.00	14.77	
ATOM	74	OD1	ASP	116	3.823	20.682	1.071	1.00	14.65	
ATOM	75	OD2	ASP	116	4.018	18.769	2.120	1.00	12.44	
ATOM	76	C	ASP	116	4.001	16.439	0.374	1.00	13.44	
ATOM	77	O	ASP	116	5.041	16.747	-0.217	1.00	13.25	
ATOM	78	N	ARG	117	3.920	15.398	1.198	1.00	10.57	
ATOM	79	CA	ARG	117	5.070	14.531	1.420	1.00	10.95	
ATOM	80	CB	ARG	117	5.415	14.453	2.916	1.00	9.63	
ATOM	81	CG	ARG	117	6.084	15.719	3.450	1.00	11.49	
ATOM	82	CD	ARG	117	6.500	15.603	4.922	1.00	11.38	
ATOM	83	NE	ARG	117	5.364	15.378	5.808	1.00	13.18	

ATOM	84	CZ	ARG	117	5.309	15.785	7.073	1.00	11.51
ATOM	85	NH1	ARG	117	6.332	16.450	7.606	1.00	10.41
ATOM	86	NH2	ARG	117	4.234	15.523	7.806	1.00	8.45
ATOM	87	C	ARG	117	4.776	13.140	0.869	1.00	11.39
ATOM	88	O	ARG	117	3.843	12.462	1.318	1.00	10.86
ATOM	89	N	SER	118	5.572	12.725	-0.112	1.00	11.70
ATOM	90	CA	SER	118	5.405	11.421	-0.738	1.00	12.38
ATOM	91	CB	SER	118	6.299	11.301	-1.977	1.00	11.70
ATOM	92	OG	SER	118	7.661	11.509	-1.644	1.00	15.48
ATOM	93	C	SER	118	5.714	10.291	0.226	1.00	12.48
ATOM	94	O	SER	118	5.332	9.146	-0.018	1.00	13.74
ATOM	95	N	THR	119	6.400	10.615	1.318	1.00	12.22
ATOM	96	CA	THR	119	6.749	9.618	2.319	1.00	11.56
ATOM	97	CB	THR	119	7.799	10.163	3.311	1.00	12.32
ATOM	98	OG1	THR	119	7.359	11.417	3.844	1.00	12.38
ATOM	99	CG2	THR	119	9.135	10.361	2.609	1.00	8.85
ATOM	100	C	THR	119	5.516	9.135	3.083	1.00	13.70
ATOM	101	O	THR	119	5.622	8.380	4.058	1.00	11.52
ATOM	102	N	VAL	120	4.342	9.585	2.649	1.00	11.86
ATOM	103	CA	VAL	120	3.107	9.130	3.265	1.00	11.85
ATOM	104	CB	VAL	120	1.871	9.844	2.658	1.00	11.66
ATOM	105	CG1	VAL	120	1.800	9.587	1.153	1.00	10.50
ATOM	106	CG2	VAL	120	0.597	9.359	3.349	1.00	11.43
ATOM	107	C	VAL	120	3.085	7.632	2.925	1.00	11.51
ATOM	108	O	VAL	120	2.362	6.844	3.535	1.00	9.54
ATOM	109	N	ARG	121	3.908	7.261	1.942	1.00	10.76
ATOM	110	CA	ARG	121	4.044	5.873	1.509	1.00	11.72
ATOM	111	CB	ARG	121	5.079	5.770	0.375	1.00	11.43
ATOM	112	CG	ARG	121	5.338	4.347	-0.129	1.00	14.00
ATOM	113	CD	ARG	121	6.479	4.308	-1.156	1.00	14.06
ATOM	114	NE	ARG	121	6.150	4.990	-2.406	1.00	16.49
ATOM	115	CZ	ARG	121	5.333	4.507	-3.335	1.00	16.27
ATOM	116	NH1	ARG	121	4.751	3.327	-3.162	1.00	16.75
ATOM	117	NH2	ARG	121	5.104	5.200	-4.445	1.00	15.29
ATOM	118	C	ARG	121	4.496	5.015	2.692	1.00	11.85
ATOM	119	O	ARG	121	3.944	3.948	2.944	1.00	10.32
ATOM	120	N	ARG	122	5.499	5.490	3.423	1.00	12.74
ATOM	121	CA	ARG	122	6.009	4.752	4.570	1.00	11.26
ATOM	122	CB	ARG	122	7.213	5.481	5.170	1.00	14.35
ATOM	123	CG	ARG	122	7.814	4.824	6.402	1.00	12.80
ATOM	124	CD	ARG	122	9.057	5.583	6.857	1.00	16.52
ATOM	125	NE	ARG	122	9.519	5.143	8.171	1.00	17.45
ATOM	126	CZ	ARG	122	10.639	5.565	8.751	1.00	20.14
ATOM	127	NH1	ARG	122	11.423	6.438	8.132	1.00	19.97
ATOM	128	NH2	ARG	122	10.969	5.125	9.960	1.00	17.32
ATOM	129	C	ARG	122	4.922	4.574	5.619	1.00	11.63
ATOM	130	O	ARG	122	4.805	3.508	6.228	1.00	8.67
ATOM	131	N	CYS	123	4.129	5.622	5.828	1.00	11.27
ATOM	132	CA	CYS	123	3.042	5.578	6.794	1.00	10.75
ATOM	133	CB	CYS	123	2.362	6.951	6.884	1.00	11.44
ATOM	134	SG	CYS	123	0.888	7.025	7.946	1.00	9.36
ATOM	135	C	CYS	123	2.027	4.521	6.372	1.00	11.83
ATOM	136	O	CYS	123	1.686	3.631	7.152	1.00	10.86
ATOM	137	N	LEU	124	1.565	4.610	5.127	1.00	11.28
ATOM	138	CA	LEU	124	0.576	3.671	4.621	1.00	10.13
ATOM	139	CB	LEU	124	0.073	4.110	3.236	1.00	10.53
ATOM	140	CG	LEU	124	-0.782	5.388	3.163	1.00	9.60
ATOM	141	CD1	LEU	124	-1.222	5.625	1.724	1.00	11.19
ATOM	142	CD2	LEU	124	-2.006	5.250	4.059	1.00	8.81
ATOM	143	C	LEU	124	1.077	2.229	4.563	1.00	10.25
ATOM	144	O	LEU	124	0.335	1.309	4.903	1.00	10.08
ATOM	145	N	ASP	125	2.324	2.021	4.141	1.00	9.94

ATOM	146	CA	ASP	125	2.847	0.660	4.068	1.00	12.02
ATOM	147	CB	ASP	125	4.315	0.642	3.620	1.00	12.22
ATOM	148	CG	ASP	125	4.488	0.985	2.144	1.00	12.03
ATOM	149	OD1	ASP	125	3.515	0.869	1.363	1.00	10.10
ATOM	150	OD2	ASP	125	5.614	1.358	1.759	1.00	10.21
ATOM	151	C	ASP	125	2.716	-0.062	5.408	1.00	12.46
ATOM	152	O	ASP	125	2.157	-1.157	5.471	1.00	11.05
ATOM	153	N	LYS	126	3.207	0.560	6.478	1.00	13.22
ATOM	154	CA	LYS	126	3.148	-0.043	7.808	1.00	14.05
ATOM	155	CB	LYS	126	3.939	0.806	8.806	1.00	16.16
ATOM	156	CG	LYS	126	5.447	0.756	8.608	1.00	17.78
ATOM	157	CD	LYS	126	5.973	-0.667	8.774	1.00	18.40
ATOM	158	CE	LYS	126	7.488	-0.728	8.639	1.00	20.47
ATOM	159	NZ	LYS	126	7.967	-0.256	7.307	1.00	19.63
ATOM	160	C	LYS	126	1.730	-0.264	8.336	1.00	13.27
ATOM	161	O	LYS	126	1.445	-1.299	8.939	1.00	14.34
ATOM	162	N	LEU	127	0.843	0.704	8.115	1.00	12.29
ATOM	163	CA	LEU	127	-0.540	0.583	8.573	1.00	12.92
ATOM	164	CB	LEU	127	-1.329	1.854	8.249	1.00	12.24
ATOM	165	CG	LEU	127	-1.200	3.065	9.169	1.00	11.93
ATOM	166	CD1	LEU	127	-1.827	4.282	8.494	1.00	11.59
ATOM	167	CD2	LEU	127	-1.887	2.779	10.493	1.00	7.66
ATOM	168	C	LEU	127	-1.231	-0.598	7.905	1.00	13.38
ATOM	169	O	LEU	127	-1.896	-1.396	8.561	1.00	14.13
ATOM	170	N	LEU	128	-1.076	-0.689	6.590	1.00	13.28
ATOM	171	CA	LEU	128	-1.686	-1.753	5.813	1.00	12.88
ATOM	172	CB	LEU	128	-1.574	-1.433	4.318	1.00	12.83
ATOM	173	CG	LEU	128	-2.528	-0.348	3.819	1.00	13.33
ATOM	174	CD1	LEU	128	-2.152	0.091	2.400	1.00	10.51
ATOM	175	CD2	LEU	128	-3.950	-0.902	3.849	1.00	12.95
ATOM	176	C	LEU	128	-1.039	-3.092	6.112	1.00	12.93
ATOM	177	O	LEU	128	-1.697	-4.131	6.077	1.00	13.55
ATOM	178	N	HIS	129	0.254	-3.067	6.410	1.00	14.18
ATOM	179	CA	HIS	129	0.968	-4.297	6.711	1.00	14.17
ATOM	180	CB	HIS	129	2.469	-4.029	6.814	1.00	16.48
ATOM	181	CG	HIS	129	3.276	-5.252	7.117	1.00	19.18
ATOM	182	CD2	HIS	129	3.794	-5.712	8.281	1.00	20.42
ATOM	183	ND1	HIS	129	3.590	-6.194	6.161	1.00	21.27
ATOM	184	CE1	HIS	129	4.266	-7.181	6.722	1.00	20.26
ATOM	185	NE2	HIS	129	4.402	-6.913	8.008	1.00	21.35
ATOM	186	C	HIS	129	0.478	-4.911	8.017	1.00	14.67
ATOM	187	O	HIS	129	0.306	-6.125	8.118	1.00	13.58
ATOM	188	N	TYR	130	0.241	-4.064	9.010	1.00	13.32
ATOM	189	CA	TYR	130	-0.198	-4.527	10.319	1.00	15.82
ATOM	190	CB	TYR	130	0.399	-3.619	11.398	1.00	15.31
ATOM	191	CG	TYR	130	1.899	-3.769	11.544	1.00	17.49
ATOM	192	CD1	TYR	130	2.724	-2.649	11.670	1.00	17.25
ATOM	193	CE1	TYR	130	4.105	-2.784	11.807	1.00	17.57
ATOM	194	CD2	TYR	130	2.494	-5.032	11.561	1.00	16.22
ATOM	195	CE2	TYR	130	3.872	-5.177	11.702	1.00	17.93
ATOM	196	CZ	TYR	130	4.671	-4.050	11.825	1.00	18.33
ATOM	197	OH	TYR	130	6.035	-4.192	11.979	1.00	20.50
ATOM	198	C	TYR	130	-1.708	-4.638	10.519	1.00	14.88
ATOM	199	O	TYR	130	-2.160	-5.339	11.419	1.00	17.33
ATOM	200	N	ARG	131	-2.486	-3.954	9.689	1.00	14.65
ATOM	201	CA	ARG	131	-3.941	-3.993	9.823	1.00	13.01
ATOM	202	CB	ARG	131	-4.601	-3.275	8.642	1.00	11.01
ATOM	203	CG	ARG	131	-6.109	-3.234	8.752	1.00	12.35
ATOM	204	CD	ARG	131	-6.733	-2.201	7.833	1.00	10.18
ATOM	205	NE	ARG	131	-6.579	-2.537	6.424	1.00	10.41
ATOM	206	CZ	ARG	131	-7.258	-1.941	5.450	1.00	11.10
ATOM	207	NH1	ARG	131	-8.133	-0.988	5.746	1.00	11.89

ATOM	208	NH2	ARG	131	-7.063	-2.292	4.184	1.00	10.83
ATOM	209	C	ARG	131	-4.457	-5.431	9.912	1.00	12.98
ATOM	210	O	ARG	131	-4.248	-6.232	9.001	1.00	12.48
ATOM	211	N	PRO	132	-5.135	-5.779	11.020	1.00	13.24
ATOM	212	CD	PRO	132	-5.222	-5.032	12.288	1.00	12.61
ATOM	213	CA	PRO	132	-5.662	-7.139	11.185	1.00	11.92
ATOM	214	CB	PRO	132	-5.773	-7.274	12.699	1.00	12.08
ATOM	215	CG	PRO	132	-6.169	-5.889	13.111	1.00	13.62
ATOM	216	C	PRO	132	-6.997	-7.387	10.490	1.00	13.75
ATOM	217	O	PRO	132	-7.404	-8.533	10.298	1.00	11.71
ATOM	218	N	SER	133	-7.679	-6.309	10.119	1.00	14.35
ATOM	219	CA	SER	133	-8.972	-6.420	9.463	1.00	15.49
ATOM	220	CB	SER	133	-10.061	-6.709	10.497	1.00	15.42
ATOM	221	OG	SER	133	-11.354	-6.562	9.933	1.00	15.51
ATOM	222	C	SER	133	-9.320	-5.143	8.727	1.00	16.44
ATOM	223	O	SER	133	-9.410	-4.079	9.337	1.00	14.24
ATOM	224	N	ALA	134	-9.531	-5.261	7.418	1.00	16.61
ATOM	225	CA	ALA	134	-9.886	-4.119	6.589	1.00	16.76
ATOM	226	CB	ALA	134	-9.891	-4.525	5.122	1.00	17.55
ATOM	227	C	ALA	134	-11.257	-3.574	6.979	1.00	17.52
ATOM	228	O	ALA	134	-11.466	-2.363	7.013	1.00	16.97
ATOM	229	N	GLU	135	-12.189	-4.476	7.273	1.00	17.67
ATOM	230	CA	GLU	135	-13.539	-4.077	7.654	1.00	19.92
ATOM	231	CB	GLU	135	-14.476	-5.293	7.691	1.00	23.25
ATOM	232	CG	GLU	135	-13.776	-6.643	7.824	1.00	29.11
ATOM	233	CD	GLU	135	-13.119	-7.089	6.528	1.00	31.07
ATOM	234	OE1	GLU	135	-13.838	-7.213	5.514	1.00	32.30
ATOM	235	OE2	GLU	135	-11.888	-7.317	6.520	1.00	31.56
ATOM	236	C	GLU	135	-13.589	-3.355	8.996	1.00	17.67
ATOM	237	O	GLU	135	-14.344	-2.401	9.162	1.00	17.07
ATOM	238	N	LEU	136	-12.786	-3.807	9.954	1.00	17.48
ATOM	239	CA	LEU	136	-12.767	-3.181	11.270	1.00	17.23
ATOM	240	CB	LEU	136	-12.177	-4.139	12.305	1.00	19.17
ATOM	241	CG	LEU	136	-13.001	-5.406	12.559	1.00	21.60
ATOM	242	CD1	LEU	136	-12.349	-6.220	13.666	1.00	19.95
ATOM	243	CD2	LEU	136	-14.429	-5.026	12.947	1.00	21.12
ATOM	244	C	LEU	136	-11.989	-1.873	11.284	1.00	16.86
ATOM	245	O	LEU	136	-12.344	-0.940	12.011	1.00	13.95
ATOM	246	N	PHE	137	-10.930	-1.806	10.479	1.00	15.80
ATOM	247	CA	PHE	137	-10.105	-0.608	10.406	1.00	13.89
ATOM	248	CB	PHE	137	-8.704	-0.884	10.962	1.00	14.28
ATOM	249	CG	PHE	137	-8.684	-1.194	12.429	1.00	17.08
ATOM	250	CD1	PHE	137	-8.824	-2.500	12.878	1.00	17.09
ATOM	251	CD2	PHE	137	-8.540	-0.172	13.365	1.00	17.81
ATOM	252	CE1	PHE	137	-8.822	-2.791	14.239	1.00	17.78
ATOM	253	CE2	PHE	137	-8.537	-0.455	14.732	1.00	17.72
ATOM	254	CZ	PHE	137	-8.678	-1.767	15.166	1.00	15.20
ATOM	255	C	PHE	137	-9.966	-0.027	9.004	1.00	12.17
ATOM	256	O	PHE	137	-8.896	-0.100	8.399	1.00	11.36
ATOM	257	N	PRO	138	-11.041	0.569	8.470	1.00	11.15
ATOM	258	CD	PRO	138	-12.379	0.789	9.043	1.00	11.29
ATOM	259	CA	PRO	138	-10.945	1.148	7.128	1.00	10.49
ATOM	260	CB	PRO	138	-12.383	1.559	6.826	1.00	8.85
ATOM	261	CG	PRO	138	-12.915	1.905	8.180	1.00	11.95
ATOM	262	C	PRO	138	-10.004	2.341	7.202	1.00	10.43
ATOM	263	O	PRO	138	-10.037	3.105	8.167	1.00	9.86
ATOM	264	N	ILE	139	-9.164	2.493	6.188	1.00	9.29
ATOM	265	CA	ILE	139	-8.207	3.590	6.154	1.00	8.30
ATOM	266	CB	ILE	139	-6.827	3.085	5.683	1.00	8.94
ATOM	267	CG2	ILE	139	-5.867	4.265	5.475	1.00	8.36
ATOM	268	CG1	ILE	139	-6.274	2.085	6.705	1.00	8.62
ATOM	269	CD1	ILE	139	-5.061	1.337	6.219	1.00	11.98

ATOM	270	C	ILE	139	-8.687	4.699	5.230	1.00	8.42
ATOM	271	O	ILE	139	-8.913	4.482	4.040	1.00	9.40
ATOM	272	N	ILE	140	-8.852	5.888	5.793	1.00	9.12
ATOM	273	CA	ILE	140	-9.294	7.040	5.026	1.00	8.73
ATOM	274	CB	ILE	140	-10.550	7.689	5.664	1.00	9.93
ATOM	275	CG2	ILE	140	-10.827	9.040	5.030	1.00	8.80
ATOM	276	CG1	ILE	140	-11.774	6.781	5.470	1.00	11.15
ATOM	277	CD1	ILE	140	-11.716	5.483	6.232	1.00	12.88
ATOM	278	C	ILE	140	-8.151	8.044	5.005	1.00	10.29
ATOM	279	O	ILE	140	-7.769	8.587	6.044	1.00	12.92
ATOM	280	N	VAL	141	-7.590	8.269	3.822	1.00	10.98
ATOM	281	CA	VAL	141	-6.488	9.210	3.664	1.00	9.42
ATOM	282	CB	VAL	141	-5.485	8.722	2.591	1.00	9.60
ATOM	283	CG1	VAL	141	-4.248	9.623	2.573	1.00	9.59
ATOM	284	CG2	VAL	141	-5.092	7.278	2.868	1.00	7.69
ATOM	285	C	VAL	141	-7.048	10.557	3.232	1.00	9.73
ATOM	286	O	VAL	141	-7.590	10.688	2.132	1.00	8.14
ATOM	287	N	SER	142	-6.942	11.555	4.102	1.00	10.38
ATOM	288	CA	SER	142	-7.433	12.887	3.770	1.00	9.24
ATOM	289	CB	SER	142	-8.121	13.528	4.977	1.00	10.29
ATOM	290	OG	SER	142	-8.802	14.719	4.604	1.00	8.99
ATOM	291	C	SER	142	-6.240	13.722	3.332	1.00	11.13
ATOM	292	O	SER	142	-5.328	13.989	4.118	1.00	11.55
ATOM	293	N	GLN	143	-6.236	14.116	2.065	1.00	8.21
ATOM	294	CA	GLN	143	-5.141	14.913	1.547	1.00	11.67
ATOM	295	CB	GLN	143	-4.583	14.312	0.254	1.00	11.04
ATOM	296	CG	GLN	143	-3.562	15.238	-0.383	1.00	13.59
ATOM	297	CD	GLN	143	-3.005	14.738	-1.692	1.00	13.39
ATOM	298	OE1	GLN	143	-3.708	14.120	-2.492	1.00	13.10
ATOM	299	NE2	GLN	143	-1.732	15.031	-1.933	1.00	13.31
ATOM	300	C	GLN	143	-5.530	16.357	1.284	1.00	11.33
ATOM	301	O	GLN	143	-6.542	16.644	0.644	1.00	12.52
ATOM	302	N	ASP	144	-4.698	17.258	1.786	1.00	11.43
ATOM	303	CA	ASP	144	-4.874	18.695	1.627	1.00	13.15
ATOM	304	CB	ASP	144	-4.720	19.354	3.009	1.00	12.32
ATOM	305	CG	ASP	144	-4.763	20.869	2.962	1.00	13.02
ATOM	306	OD1	ASP	144	-5.517	21.431	2.148	1.00	10.17
ATOM	307	OD2	ASP	144	-4.051	21.504	3.771	1.00	15.63
ATOM	308	C	ASP	144	-3.738	19.103	0.685	1.00	12.80
ATOM	309	O	ASP	144	-2.979	18.242	0.232	1.00	11.31
ATOM	310	N	CYS	145	-3.648	20.387	0.355	1.00	12.66
ATOM	311	CA	CYS	145	-2.551	20.886	-0.472	1.00	14.95
ATOM	312	C	CYS	145	-2.547	20.613	-1.976	1.00	17.15
ATOM	313	O	CYS	145	-1.931	21.361	-2.729	1.00	18.08
ATOM	314	CB	CYS	145	-1.240	20.390	0.135	1.00	14.83
ATOM	315	SG	CYS	145	-1.194	20.704	1.928	1.00	16.85
ATOM	316	N	GLY	146	-3.202	19.545	-2.416	1.00	16.70
ATOM	317	CA	GLY	146	-3.231	19.247	-3.840	1.00	18.47
ATOM	318	C	GLY	146	-1.888	18.925	-4.485	1.00	18.78
ATOM	319	O	GLY	146	-1.667	19.246	-5.652	1.00	19.92
ATOM	320	N	HIS	147	-0.992	18.290	-3.735	1.00	17.06
ATOM	321	CA	HIS	147	0.329	17.917	-4.243	1.00	16.44
ATOM	322	CB	HIS	147	1.242	17.570	-3.056	1.00	15.10
ATOM	323	CG	HIS	147	2.682	17.369	-3.418	1.00	13.87
ATOM	324	CD2	HIS	147	3.686	18.259	-3.609	1.00	15.01
ATOM	325	ND1	HIS	147	3.244	16.120	-3.579	1.00	12.64
ATOM	326	CE1	HIS	147	4.531	16.248	-3.850	1.00	11.35
ATOM	327	NE2	HIS	147	4.825	17.536	-3.875	1.00	10.77
ATOM	328	C	HIS	147	0.134	16.706	-5.155	1.00	17.16
ATOM	329	O	HIS	147	-0.172	15.615	-4.681	1.00	16.72
ATOM	330	N	GLU	148	0.316	16.906	-6.459	1.00	17.38
ATOM	331	CA	GLU	148	0.120	15.845	-7.451	1.00	18.49

ATOM	332	CB	GLU	148	0.507	16.351	-8.845	1.00	21.96
ATOM	333	CG	GLU	148	0.233	15.361	-9.970	1.00	26.31
ATOM	334	CD	GLU	148	-1.219	14.918	-10.020	1.00	31.03
ATOM	335	OE1	GLU	148	-2.110	15.789	-9.912	1.00	33.63
ATOM	336	OE2	GLU	148	-1.472	13.701	-10.176	1.00	32.66
ATOM	337	C	GLU	148	0.843	14.526	-7.179	1.00	17.23
ATOM	338	O	GLU	148	0.223	13.463	-7.200	1.00	16.11
ATOM	339	N	GLU	149	2.147	14.586	-6.936	1.00	15.28
ATOM	340	CA	GLU	149	2.903	13.368	-6.680	1.00	17.49
ATOM	341	CB	GLU	149	4.387	13.681	-6.507	1.00	20.21
ATOM	342	CG	GLU	149	5.222	12.466	-6.168	1.00	22.65
ATOM	343	CD	GLU	149	6.697	12.789	-6.082	1.00	25.52
ATOM	344	OE1	GLU	149	7.457	11.978	-5.511	1.00	26.66
ATOM	345	OE2	GLU	149	7.094	13.855	-6.594	1.00	29.34
ATOM	346	C	GLU	149	2.389	12.630	-5.451	1.00	16.77
ATOM	347	O	GLU	149	2.257	11.407	-5.463	1.00	16.67
ATOM	348	N	THR	150	2.104	13.368	-4.385	1.00	16.42
ATOM	349	CA	THR	150	1.600	12.733	-3.178	1.00	14.69
ATOM	350	CB	THR	150	1.460	13.741	-2.024	1.00	13.84
ATOM	351	OG1	THR	150	2.751	14.287	-1.702	1.00	11.52
ATOM	352	CG2	THR	150	0.898	13.044	-0.786	1.00	13.95
ATOM	353	C	THR	150	0.236	12.118	-3.490	1.00	13.83
ATOM	354	O	THR	150	-0.121	11.071	-2.948	1.00	16.52
ATOM	355	N	ALA	151	-0.515	12.769	-4.376	1.00	13.24
ATOM	356	CA	ALA	151	-1.832	12.279	-4.765	1.00	10.86
ATOM	357	CB	ALA	151	-2.547	13.321	-5.624	1.00	12.74
ATOM	358	C	ALA	151	-1.707	10.963	-5.531	1.00	13.05
ATOM	359	O	ALA	151	-2.488	10.032	-5.311	1.00	11.92
ATOM	360	N	GLN	152	-0.725	10.890	-6.429	1.00	13.63
ATOM	361	CA	GLN	152	-0.501	9.679	-7.227	1.00	15.48
ATOM	362	CB	GLN	152	0.679	9.868	-8.185	1.00	18.54
ATOM	363	CG	GLN	152	0.713	11.203	-8.903	1.00	22.92
ATOM	364	CD	GLN	152	-0.233	11.272	-10.077	1.00	27.51
ATOM	365	OE1	GLN	152	-1.442	11.060	-9.936	1.00	31.13
ATOM	366	NE2	GLN	152	0.311	11.581	-11.253	1.00	28.72
ATOM	367	C	GLN	152	-0.170	8.533	-6.281	1.00	14.42
ATOM	368	O	GLN	152	-0.737	7.446	-6.374	1.00	16.73
ATOM	369	N	VAL	153	0.767	8.790	-5.377	1.00	11.61
ATOM	370	CA	VAL	153	1.198	7.801	-4.400	1.00	10.62
ATOM	371	CB	VAL	153	2.181	8.423	-3.393	1.00	12.39
ATOM	372	CG1	VAL	153	2.528	7.412	-2.296	1.00	11.24
ATOM	373	CG2	VAL	153	3.437	8.881	-4.127	1.00	13.55
ATOM	374	C	VAL	153	0.023	7.211	-3.633	1.00	9.14
ATOM	375	O	VAL	153	-0.085	5.988	-3.492	1.00	9.69
ATOM	376	N	ILE	154	-0.856	8.080	-3.144	1.00	7.74
ATOM	377	CA	ILE	154	-2.016	7.635	-2.391	1.00	9.09
ATOM	378	CB	ILE	154	-2.805	8.834	-1.804	1.00	6.62
ATOM	379	CG2	ILE	154	-4.030	8.335	-1.058	1.00	2.85
ATOM	380	CG1	ILE	154	-1.912	9.627	-0.841	1.00	7.01
ATOM	381	CD1	ILE	154	-2.533	10.928	-0.307	1.00	5.64
ATOM	382	C	ILE	154	-2.913	6.820	-3.313	1.00	10.32
ATOM	383	O	ILE	154	-3.344	5.728	-2.957	1.00	11.90
ATOM	384	N	ALA	155	-3.169	7.348	-4.508	1.00	12.08
ATOM	385	CA	ALA	155	-4.012	6.677	-5.497	1.00	13.34
ATOM	386	CB	ALA	155	-4.124	7.539	-6.755	1.00	14.73
ATOM	387	C	ALA	155	-3.498	5.286	-5.875	1.00	13.81
ATOM	388	O	ALA	155	-4.289	4.389	-6.170	1.00	12.64
ATOM	389	N	SER	156	-2.178	5.108	-5.871	1.00	13.37
ATOM	390	CA	SER	156	-1.589	3.824	-6.233	1.00	13.26
ATOM	391	CB	SER	156	-0.058	3.924	-6.286	1.00	12.56
ATOM	392	OG	SER	156	0.530	3.865	-4.995	1.00	11.28
ATOM	393	C	SER	156	-1.996	2.684	-5.299	1.00	14.35

ATOM	394	O	SER	156	-1.793	1.512	-5.626	1.00	15.79
ATOM	395	N	TYR	157	-2.561	3.011	-4.139	1.00	13.36
ATOM	396	CA	TYR	157	-2.993	1.967	-3.214	1.00	13.45
ATOM	397	CB	TYR	157	-3.033	2.484	-1.773	1.00	13.13
ATOM	398	CG	TYR	157	-1.661	2.652	-1.177	1.00	11.58
ATOM	399	CD1	TYR	157	-0.879	3.761	-1.482	1.00	11.70
ATOM	400	CE1	TYR	157	0.413	3.900	-0.967	1.00	10.82
ATOM	401	CD2	TYR	157	-1.123	1.676	-0.337	1.00	12.65
ATOM	402	CE2	TYR	157	0.165	1.801	0.182	1.00	12.15
ATOM	403	CZ	TYR	157	0.928	2.917	-0.139	1.00	12.65
ATOM	404	OH	TYR	157	2.208	3.034	0.366	1.00	13.62
ATOM	405	C	TYR	157	-4.358	1.418	-3.604	1.00	13.47
ATOM	406	O	TYR	157	-4.810	0.408	-3.066	1.00	13.88
ATOM	407	N	GLY	158	-5.011	2.086	-4.547	1.00	12.50
ATOM	408	CA	GLY	158	-6.313	1.631	-4.994	1.00	13.92
ATOM	409	C	GLY	158	-7.315	1.430	-3.872	1.00	13.99
ATOM	410	O	GLY	158	-7.434	2.269	-2.978	1.00	14.76
ATOM	411	N	SER	159	-8.026	0.307	-3.921	1.00	15.36
ATOM	412	CA	SER	159	-9.054	-0.028	-2.932	1.00	16.25
ATOM	413	CB	SER	159	-9.767	-1.321	-3.333	1.00	17.73
ATOM	414	OG	SER	159	-8.886	-2.434	-3.283	1.00	25.56
ATOM	415	C	SER	159	-8.573	-0.174	-1.493	1.00	14.50
ATOM	416	O	SER	159	-9.385	-0.182	-0.571	1.00	14.26
ATOM	417	N	ALA	160	-7.267	-0.299	-1.292	1.00	13.67
ATOM	418	CA	ALA	160	-6.740	-0.452	0.058	1.00	13.13
ATOM	419	CB	ALA	160	-5.226	-0.650	0.014	1.00	13.61
ATOM	420	C	ALA	160	-7.096	0.751	0.935	1.00	13.61
ATOM	421	O	ALA	160	-7.174	0.632	2.161	1.00	15.00
ATOM	422	N	VAL	161	-7.319	1.906	0.311	1.00	12.23
ATOM	423	CA	VAL	161	-7.672	3.104	1.066	1.00	12.14
ATOM	424	CB	VAL	161	-6.443	4.026	1.285	1.00	13.71
ATOM	425	CG1	VAL	161	-5.355	3.283	2.032	1.00	12.34
ATOM	426	CG2	VAL	161	-5.926	4.531	-0.064	1.00	12.47
ATOM	427	C	VAL	161	-8.738	3.932	0.371	1.00	13.09
ATOM	428	O	VAL	161	-9.085	3.684	-0.786	1.00	14.34
ATOM	429	N	THR	162	-9.259	4.916	1.096	1.00	12.82
ATOM	430	CA	THR	162	-10.250	5.831	0.563	1.00	13.16
ATOM	431	CB	THR	162	-11.512	5.903	1.457	1.00	12.58
ATOM	432	OG1	THR	162	-12.194	4.642	1.429	1.00	12.51
ATOM	433	CG2	THR	162	-12.459	6.990	0.954	1.00	13.56
ATOM	434	C	THR	162	-9.544	7.183	0.552	1.00	13.69
ATOM	435	O	THR	162	-9.173	7.708	1.604	1.00	12.63
ATOM	436	N	HIS	163	-9.348	7.732	-0.643	1.00	11.38
ATOM	437	CA	HIS	163	-8.659	9.006	-0.805	1.00	12.04
ATOM	438	CB	HIS	163	-7.783	8.944	-2.067	1.00	10.81
ATOM	439	CG	HIS	163	-6.848	10.103	-2.225	1.00	11.90
ATOM	440	CD2	HIS	163	-6.474	11.076	-1.360	1.00	12.29
ATOM	441	ND1	HIS	163	-6.154	10.343	-3.393	1.00	11.89
ATOM	442	CE1	HIS	163	-5.397	11.415	-3.242	1.00	9.73
ATOM	443	NE2	HIS	163	-5.572	11.879	-2.017	1.00	14.87
ATOM	444	C	HIS	163	-9.645	10.167	-0.920	1.00	11.03
ATOM	445	O	HIS	163	-10.445	10.205	-1.857	1.00	11.78
ATOM	446	N	ILE	164	-9.610	11.091	0.039	1.00	11.12
ATOM	447	CA	ILE	164	-10.481	12.263	0.000	1.00	10.46
ATOM	448	CB	ILE	164	-11.466	12.323	1.206	1.00	10.12
ATOM	449	CG2	ILE	164	-12.428	11.145	1.131	1.00	8.15
ATOM	450	CG1	ILE	164	-10.703	12.342	2.530	1.00	10.01
ATOM	451	CD1	ILE	164	-11.593	12.577	3.747	1.00	10.40
ATOM	452	C	ILE	164	-9.606	13.510	-0.020	1.00	11.95
ATOM	453	O	ILE	164	-8.490	13.514	0.517	1.00	11.72
ATOM	454	N	ARG	165	-10.110	14.568	-0.641	1.00	11.72
ATOM	455	CA	ARG	165	-9.334	15.792	-0.772	1.00	12.98

ATOM	456	CB	ARG	165	-9.019	16.018	-2.250	1.00	13.70
ATOM	457	CG	ARG	165	-8.382	14.806	-2.909	1.00	15.54
ATOM	458	CD	ARG	165	-8.058	15.049	-4.371	1.00	22.22
ATOM	459	NE	ARG	165	-7.533	13.838	-4.999	1.00	25.48
ATOM	460	CZ	ARG	165	-6.918	13.807	-6.179	1.00	27.50
ATOM	461	NH1	ARG	165	-6.743	14.925	-6.871	1.00	27.83
ATOM	462	NH2	ARG	165	-6.471	12.654	-6.664	1.00	27.97
ATOM	463	C	ARG	165	-9.985	17.034	-0.190	1.00	12.35
ATOM	464	O	ARG	165	-11.111	17.390	-0.550	1.00	13.45
ATOM	465	N	GLN	166	-9.261	17.686	0.717	1.00	10.50
ATOM	466	CA	GLN	166	-9.732	18.908	1.350	1.00	10.77
ATOM	467	CB	GLN	166	-8.617	19.482	2.229	1.00	10.64
ATOM	468	CG	GLN	166	-9.083	20.426	3.324	1.00	10.96
ATOM	469	CD	GLN	166	-9.348	21.820	2.808	1.00	11.15
ATOM	470	OE1	GLN	166	-10.499	22.235	2.637	1.00	8.80
ATOM	471	NE2	GLN	166	-8.274	22.555	2.544	1.00	10.58
ATOM	472	C	GLN	166	-10.058	19.816	0.161	1.00	10.44
ATOM	473	O	GLN	166	-9.214	20.049	-0.699	1.00	7.01
ATOM	474	N	PRO	167	-11.296	20.325	0.094	1.00	11.20
ATOM	475	CD	PRO	167	-12.387	20.064	1.053	1.00	10.78
ATOM	476	CA	PRO	167	-11.757	21.189	-0.998	1.00	13.01
ATOM	477	CB	PRO	167	-13.272	21.051	-0.908	1.00	11.00
ATOM	478	CG	PRO	167	-13.489	20.998	0.572	1.00	12.17
ATOM	479	C	PRO	167	-11.327	22.650	-1.084	1.00	15.30
ATOM	480	O	PRO	167	-11.417	23.247	-2.156	1.00	19.24
ATOM	481	N	ASP	168	-10.858	23.233	0.013	1.00	15.86
ATOM	482	CA	ASP	168	-10.474	24.641	-0.007	1.00	16.33
ATOM	483	CB	ASP	168	-11.182	25.367	1.139	1.00	17.66
ATOM	484	CG	ASP	168	-11.052	26.868	1.043	1.00	19.95
ATOM	485	OD1	ASP	168	-10.783	27.360	-0.069	1.00	21.44
ATOM	486	OD2	ASP	168	-11.232	27.553	2.074	1.00	22.08
ATOM	487	C	ASP	168	-8.967	24.859	0.076	1.00	16.53
ATOM	488	O	ASP	168	-8.378	24.782	1.153	1.00	16.38
ATOM	489	N	LEU	169	-8.347	25.144	-1.067	1.00	17.30
ATOM	490	CA	LEU	169	-6.905	25.347	-1.115	1.00	18.26
ATOM	491	CB	LEU	169	-6.319	24.632	-2.336	1.00	18.09
ATOM	492	CG	LEU	169	-6.562	23.119	-2.340	1.00	20.47
ATOM	493	CD1	LEU	169	-5.812	22.471	-3.490	1.00	21.27
ATOM	494	CD2	LEU	169	-6.100	22.530	-1.015	1.00	19.51
ATOM	495	C	LEU	169	-6.466	26.805	-1.117	1.00	19.32
ATOM	496	O	LEU	169	-5.299	27.104	-1.371	1.00	20.00
ATOM	497	N	SER	170	-7.390	27.709	-0.822	1.00	18.09
ATOM	498	CA	SER	170	-7.072	29.132	-0.804	1.00	18.32
ATOM	499	CB	SER	170	-8.352	29.953	-0.644	1.00	18.40
ATOM	500	OG	SER	170	-8.899	29.758	0.648	1.00	18.58
ATOM	501	C	SER	170	-6.131	29.462	0.347	1.00	17.80
ATOM	502	O	SER	170	-6.027	28.705	1.309	1.00	17.11
ATOM	503	N	ASN	171	-5.436	30.589	0.248	1.00	17.67
ATOM	504	CA	ASN	171	-4.548	30.991	1.326	1.00	18.61
ATOM	505	CB	ASN	171	-3.583	32.090	0.878	1.00	20.86
ATOM	506	CG	ASN	171	-2.497	31.570	-0.039	1.00	23.21
ATOM	507	OD1	ASN	171	-1.957	30.480	0.174	1.00	24.06
ATOM	508	ND2	ASN	171	-2.158	32.350	-1.058	1.00	25.07
ATOM	509	C	ASN	171	-5.419	31.497	2.460	1.00	18.38
ATOM	510	O	ASN	171	-6.557	31.923	2.246	1.00	18.60
ATOM	511	N	ILE	172	-4.886	31.455	3.671	1.00	17.06
ATOM	512	CA	ILE	172	-5.642	31.892	4.826	1.00	17.00
ATOM	513	CB	ILE	172	-5.617	30.801	5.919	1.00	14.20
ATOM	514	CG2	ILE	172	-6.355	31.275	7.161	1.00	14.59
ATOM	515	CG1	ILE	172	-6.262	29.525	5.367	1.00	14.75
ATOM	516	CD1	ILE	172	-6.303	28.373	6.339	1.00	12.84
ATOM	517	C	ILE	172	-5.131	33.214	5.382	1.00	17.59

ATOM	518	O	ILE	172	-3.922	33.419	5.521	1.00	18.11
ATOM	519	N	ALA	173	-6.063	34.115	5.679	1.00	17.91
ATOM	520	CA	ALA	173	-5.718	35.418	6.233	1.00	18.28
ATOM	521	CB	ALA	173	-6.883	36.390	6.055	1.00	18.83
ATOM	522	C	ALA	173	-5.407	35.234	7.714	1.00	17.30
ATOM	523	O	ALA	173	-6.303	34.996	8.516	1.00	18.88
ATOM	524	N	VAL	174	-4.132	35.347	8.071	1.00	16.16
ATOM	525	CA	VAL	174	-3.712	35.179	9.454	1.00	13.50
ATOM	526	CB	VAL	174	-2.251	34.671	9.522	1.00	11.32
ATOM	527	CG1	VAL	174	-2.124	33.335	8.791	1.00	11.75
ATOM	528	CG2	VAL	174	-1.314	35.703	8.896	1.00	12.19
ATOM	529	C	VAL	174	-3.817	36.477	10.256	1.00	14.14
ATOM	530	O	VAL	174	-3.960	37.563	9.694	1.00	12.74
ATOM	531	N	GLN	175	-3.767	36.354	11.577	1.00	14.74
ATOM	532	CA	GLN	175	-3.825	37.520	12.441	1.00	14.72
ATOM	533	CB	GLN	175	-4.177	37.098	13.871	1.00	14.97
ATOM	534	CG	GLN	175	-5.654	36.766	14.052	1.00	15.14
ATOM	535	CD	GLN	175	-6.540	37.992	13.915	1.00	17.21
ATOM	536	OE1	GLN	175	-6.390	38.958	14.659	1.00	17.63
ATOM	537	NE2	GLN	175	-7.466	37.958	12.962	1.00	18.51
ATOM	538	C	GLN	175	-2.467	38.220	12.377	1.00	15.18
ATOM	539	O	GLN	175	-1.479	37.627	11.933	1.00	15.34
ATOM	540	N	PRO	176	-2.402	39.491	12.811	1.00	14.90
ATOM	541	CD	PRO	176	-3.506	40.246	13.427	1.00	15.17
ATOM	542	CA	PRO	176	-1.173	40.298	12.802	1.00	16.01
ATOM	543	CB	PRO	176	-1.587	41.566	13.547	1.00	15.13
ATOM	544	CG	PRO	176	-3.047	41.671	13.250	1.00	15.80
ATOM	545	C	PRO	176	0.055	39.654	13.431	1.00	15.89
ATOM	546	O	PRO	176	1.184	39.993	13.085	1.00	17.74
ATOM	547	N	ASP	177	-0.162	38.727	14.355	1.00	16.66
ATOM	548	CA	ASP	177	0.942	38.069	15.042	1.00	15.89
ATOM	549	CB	ASP	177	0.564	37.864	16.516	1.00	15.24
ATOM	550	CG	ASP	177	-0.672	36.985	16.697	1.00	16.55
ATOM	551	OD1	ASP	177	-1.597	37.041	15.853	1.00	16.73
ATOM	552	OD2	ASP	177	-0.730	36.243	17.701	1.00	15.02
ATOM	553	C	ASP	177	1.375	36.735	14.437	1.00	16.77
ATOM	554	O	ASP	177	2.333	36.124	14.908	1.00	15.66
ATOM	555	N	HIS	178	0.703	36.302	13.374	1.00	15.66
ATOM	556	CA	HIS	178	1.002	35.001	12.778	1.00	13.48
ATOM	557	CB	HIS	178	-0.237	34.115	12.911	1.00	13.61
ATOM	558	CG	HIS	178	-0.622	33.824	14.331	1.00	12.26
ATOM	559	CD2	HIS	178	0.121	33.747	15.459	1.00	10.15
ATOM	560	ND1	HIS	178	-1.912	33.506	14.700	1.00	10.96
ATOM	561	CE1	HIS	178	-1.945	33.243	15.994	1.00	13.29
ATOM	562	NE2	HIS	178	-0.724	33.381	16.478	1.00	13.41
ATOM	563	C	HIS	178	1.493	34.962	11.332	1.00	13.60
ATOM	564	O	HIS	178	1.293	33.967	10.635	1.00	11.39
ATOM	565	N	ARG	179	2.158	36.019	10.886	1.00	12.87
ATOM	566	CA	ARG	179	2.654	36.067	9.511	1.00	16.29
ATOM	567	CB	ARG	179	3.507	37.322	9.303	1.00	19.29
ATOM	568	CG	ARG	179	3.223	38.048	7.998	1.00	26.37
ATOM	569	CD	ARG	179	1.856	38.729	8.023	1.00	28.75
ATOM	570	NE	ARG	179	1.796	39.809	9.009	1.00	30.87
ATOM	571	CZ	ARG	179	0.730	40.580	9.215	1.00	30.91
ATOM	572	NH1	ARG	179	-0.376	40.396	8.505	1.00	29.58
ATOM	573	NH2	ARG	179	0.770	41.539	10.132	1.00	29.29
ATOM	574	C	ARG	179	3.478	34.828	9.155	1.00	15.91
ATOM	575	O	ARG	179	3.378	34.295	8.048	1.00	15.09
ATOM	576	N	LYS	180	4.285	34.369	10.103	1.00	15.10
ATOM	577	CA	LYS	180	5.137	33.208	9.881	1.00	16.96
ATOM	578	CB	LYS	180	6.425	33.351	10.699	1.00	17.16
ATOM	579	CG	LYS	180	7.122	34.698	10.520	1.00	20.45

ATOM	580	CD	LYS	180	8.512	34.737	11.149	1.00	22.90
ATOM	581	CE	LYS	180	8.481	34.485	12.650	1.00	24.12
ATOM	582	NZ	LYS	180	8.080	33.085	12.968	1.00	24.84
ATOM	583	C	LYS	180	4.481	31.868	10.216	1.00	16.39
ATOM	584	O	LYS	180	5.134	30.830	10.149	1.00	17.95
ATOM	585	N	PHE	181	3.196	31.869	10.549	1.00	16.19
ATOM	586	CA	PHE	181	2.552	30.613	10.918	1.00	15.57
ATOM	587	CB	PHE	181	2.221	30.625	12.414	1.00	16.62
ATOM	588	CG	PHE	181	3.381	31.012	13.288	1.00	18.09
ATOM	589	CD1	PHE	181	3.570	32.337	13.670	1.00	18.89
ATOM	590	CD2	PHE	181	4.299	30.057	13.713	1.00	18.90
ATOM	591	CE1	PHE	181	4.655	32.704	14.462	1.00	18.52
ATOM	592	CE2	PHE	181	5.388	30.416	14.505	1.00	18.47
ATOM	593	CZ	PHE	181	5.565	31.743	14.879	1.00	18.84
ATOM	594	C	PHE	181	1.302	30.224	10.136	1.00	16.18
ATOM	595	O	PHE	181	0.422	29.559	10.678	1.00	14.26
ATOM	596	N	GLN	182	1.220	30.614	8.867	1.00	17.10
ATOM	597	CA	GLN	182	0.047	30.263	8.080	1.00	17.98
ATOM	598	CB	GLN	182	0.100	30.911	6.692	1.00	18.89
ATOM	599	CG	GLN	182	-1.163	30.651	5.881	1.00	22.36
ATOM	600	CD	GLN	182	-1.282	31.531	4.658	1.00	24.18
ATOM	601	OE1	GLN	182	-2.224	31.394	3.877	1.00	28.32
ATOM	602	NE2	GLN	182	-0.333	32.445	4.483	1.00	25.41
ATOM	603	C	GLN	182	-0.076	28.747	7.942	1.00	17.11
ATOM	604	O	GLN	182	-1.176	28.217	7.799	1.00	17.10
ATOM	605	N	GLY	183	1.057	28.050	7.982	1.00	16.21
ATOM	606	CA	GLY	183	1.022	26.604	7.873	1.00	15.88
ATOM	607	C	GLY	183	0.144	25.996	8.952	1.00	15.22
ATOM	608	O	GLY	183	-0.596	25.042	8.702	1.00	16.15
ATOM	609	N	TYR	184	0.222	26.546	10.161	1.00	15.48
ATOM	610	CA	TYR	184	-0.585	26.043	11.270	1.00	12.67
ATOM	611	CB	TYR	184	-0.124	26.664	12.587	1.00	12.35
ATOM	612	CG	TYR	184	1.296	26.292	12.938	1.00	13.70
ATOM	613	CD1	TYR	184	2.361	27.123	12.593	1.00	14.40
ATOM	614	CE1	TYR	184	3.679	26.758	12.866	1.00	16.85
ATOM	615	CD2	TYR	184	1.580	25.086	13.568	1.00	14.82
ATOM	616	CE2	TYR	184	2.894	24.707	13.843	1.00	17.76
ATOM	617	CZ	TYR	184	3.936	25.547	13.489	1.00	18.28
ATOM	618	OH	TYR	184	5.232	25.172	13.751	1.00	19.90
ATOM	619	C	TYR	184	-2.076	26.301	11.056	1.00	11.99
ATOM	620	O	TYR	184	-2.917	25.540	11.541	1.00	12.05
ATOM	621	N	TYR	185	-2.403	27.376	10.341	1.00	10.38
ATOM	622	CA	TYR	185	-3.797	27.696	10.055	1.00	10.40
ATOM	623	CB	TYR	185	-3.925	29.074	9.392	1.00	9.15
ATOM	624	CG	TYR	185	-3.911	30.247	10.351	1.00	9.22
ATOM	625	CD1	TYR	185	-2.775	30.550	11.107	1.00	8.38
ATOM	626	CE1	TYR	185	-2.761	31.636	11.978	1.00	8.08
ATOM	627	CD2	TYR	185	-5.036	31.063	10.494	1.00	8.14
ATOM	628	CE2	TYR	185	-5.031	32.150	11.362	1.00	7.60
ATOM	629	CZ	TYR	185	-3.892	32.429	12.100	1.00	6.51
ATOM	630	OH	TYR	185	-3.893	33.494	12.970	1.00	6.96
ATOM	631	C	TYR	185	-4.331	26.635	9.097	1.00	12.16
ATOM	632	O	TYR	185	-5.465	26.163	9.231	1.00	15.05
ATOM	633	N	LYS	186	-3.505	26.267	8.122	1.00	12.27
ATOM	634	CA	LYS	186	-3.894	25.269	7.138	1.00	10.86
ATOM	635	CB	LYS	186	-2.844	25.201	6.021	1.00	12.95
ATOM	636	CG	LYS	186	-2.728	26.519	5.254	1.00	16.81
ATOM	637	CD	LYS	186	-1.868	26.418	4.008	1.00	19.43
ATOM	638	CE	LYS	186	-1.911	27.733	3.233	1.00	22.79
ATOM	639	NZ	LYS	186	-1.136	27.692	1.965	1.00	24.06
ATOM	640	C	LYS	186	-4.097	23.908	7.794	1.00	10.01
ATOM	641	O	LYS	186	-5.025	23.176	7.435	1.00	9.18

ATOM	642	N	ILE	187	-3.251	23.577	8.772	1.00	10.39
ATOM	643	CA	ILE	187	-3.371	22.300	9.475	1.00	10.32
ATOM	644	CB	ILE	187	-2.224	22.094	10.509	1.00	9.67
ATOM	645	CG2	ILE	187	-2.486	20.843	11.338	1.00	13.32
ATOM	646	CG1	ILE	187	-0.878	21.970	9.786	1.00	11.84
ATOM	647	CD1	ILE	187	0.320	21.811	10.720	1.00	12.05
ATOM	648	C	ILE	187	-4.709	22.245	10.213	1.00	9.48
ATOM	649	O	ILE	187	-5.446	21.259	10.114	1.00	8.53
ATOM	650	N	ALA	188	-5.031	23.306	10.947	1.00	10.07
ATOM	651	CA	ALA	188	-6.288	23.336	11.686	1.00	10.10
ATOM	652	CB	ALA	188	-6.398	24.630	12.486	1.00	9.44
ATOM	653	C	ALA	188	-7.472	23.190	10.737	1.00	10.74
ATOM	654	O	ALA	188	-8.352	22.353	10.957	1.00	10.87
ATOM	655	N	ARG	189	-7.491	23.994	9.675	1.00	9.39
ATOM	656	CA	ARG	189	-8.573	23.925	8.697	1.00	9.38
ATOM	657	CB	ARG	189	-8.320	24.877	7.520	1.00	10.32
ATOM	658	CG	ARG	189	-9.311	24.689	6.375	1.00	8.69
ATOM	659	CD	ARG	189	-9.119	25.737	5.284	1.00	8.89
ATOM	660	NE	ARG	189	-7.841	25.584	4.594	1.00	10.83
ATOM	661	CZ	ARG	189	-7.391	26.426	3.670	1.00	9.34
ATOM	662	NH1	ARG	189	-8.118	27.483	3.330	1.00	11.15
ATOM	663	NH2	ARG	189	-6.222	26.210	3.083	1.00	7.29
ATOM	664	C	ARG	189	-8.745	22.509	8.160	1.00	9.42
ATOM	665	O	ARG	189	-9.872	22.020	8.048	1.00	11.03
ATOM	666	N	HIS	190	-7.634	21.849	7.827	1.00	8.29
ATOM	667	CA	HIS	190	-7.706	20.485	7.306	1.00	8.31
ATOM	668	CB	HIS	190	-6.326	19.973	6.877	1.00	9.24
ATOM	669	CG	HIS	190	-6.370	18.659	6.154	1.00	8.20
ATOM	670	CD2	HIS	190	-7.407	17.972	5.616	1.00	9.15
ATOM	671	ND1	HIS	190	-5.241	17.913	5.890	1.00	8.67
ATOM	672	CE1	HIS	190	-5.579	16.824	5.222	1.00	9.43
ATOM	673	NE2	HIS	190	-6.888	16.836	5.041	1.00	9.08
ATOM	674	C	HIS	190	-8.293	19.534	8.342	1.00	8.73
ATOM	675	O	HIS	190	-9.171	18.729	8.021	1.00	8.85
ATOM	676	N	TYR	191	-7.809	19.614	9.579	1.00	6.70
ATOM	677	CA	TYR	191	-8.326	18.753	10.638	1.00	8.91
ATOM	678	CB	TYR	191	-7.660	19.064	11.978	1.00	8.99
ATOM	679	CG	TYR	191	-6.465	18.197	12.267	1.00	7.73
ATOM	680	CD1	TYR	191	-5.309	18.291	11.492	1.00	6.68
ATOM	681	CE1	TYR	191	-4.206	17.490	11.755	1.00	9.22
ATOM	682	CD2	TYR	191	-6.488	17.279	13.320	1.00	6.30
ATOM	683	CE2	TYR	191	-5.390	16.476	13.594	1.00	8.34
ATOM	684	CZ	TYR	191	-4.252	16.584	12.807	1.00	8.56
ATOM	685	OH	TYR	191	-3.167	15.777	13.061	1.00	9.48
ATOM	686	C	TYR	191	-9.831	18.908	10.789	1.00	9.69
ATOM	687	O	TYR	191	-10.552	17.920	10.930	1.00	7.02
ATOM	688	N	ARG	192	-10.314	20.146	10.765	1.00	11.20
ATOM	689	CA	ARG	192	-11.746	20.356	10.906	1.00	11.66
ATOM	690	CB	ARG	192	-12.091	21.846	10.917	1.00	17.08
ATOM	691	CG	ARG	192	-13.592	22.092	10.997	1.00	21.13
ATOM	692	CD	ARG	192	-13.958	23.564	10.999	1.00	27.20
ATOM	693	NE	ARG	192	-13.981	24.137	12.342	1.00	32.04
ATOM	694	CZ	ARG	192	-14.626	25.258	12.659	1.00	33.72
ATOM	695	NH1	ARG	192	-15.298	25.920	11.724	1.00	33.92
ATOM	696	NH2	ARG	192	-14.606	25.716	13.905	1.00	33.19
ATOM	697	C	ARG	192	-12.498	19.660	9.774	1.00	11.43
ATOM	698	O	ARG	192	-13.443	18.917	10.018	1.00	9.07
ATOM	699	N	TRP	193	-12.074	19.890	8.536	1.00	11.45
ATOM	700	CA	TRP	193	-12.738	19.265	7.400	1.00	12.53
ATOM	701	CB	TRP	193	-12.152	19.770	6.075	1.00	10.59
ATOM	702	CG	TRP	193	-12.885	19.218	4.878	1.00	10.86
ATOM	703	CD2	TRP	193	-12.529	18.060	4.111	1.00	11.31

ATOM	704	CE2	TRP	193	-13.536	17.878	3.133	1.00	10.99
ATOM	705	CE3	TRP	193	-11.460	17.157	4.156	1.00	9.45
ATOM	706	CD1	TRP	193	-14.058	19.678	4.347	1.00	12.31
ATOM	707	NE1	TRP	193	-14.454	18.879	3.300	1.00	12.70
ATOM	708	CZ2	TRP	193	-13.503	16.829	2.205	1.00	11.59
ATOM	709	CZ3	TRP	193	-11.426	16.110	3.230	1.00	10.27
ATOM	710	CH2	TRP	193	-12.445	15.959	2.268	1.00	12.80
ATOM	711	C	TRP	193	-12.636	17.738	7.434	1.00	13.03
ATOM	712	O	TRP	193	-13.638	17.037	7.243	1.00	12.87
ATOM	713	N	ALA	194	-11.428	17.229	7.677	1.00	12.35
ATOM	714	CA	ALA	194	-11.187	15.786	7.714	1.00	11.00
ATOM	715	CB	ALA	194	-9.692	15.507	7.890	1.00	10.88
ATOM	716	C	ALA	194	-11.980	15.080	8.807	1.00	11.74
ATOM	717	O	ALA	194	-12.576	14.031	8.566	1.00	12.38
ATOM	718	N	LEU	195	-11.982	15.639	10.012	1.00	10.05
ATOM	719	CA	LEU	195	-12.730	15.019	11.097	1.00	11.64
ATOM	720	CB	LEU	195	-12.352	15.662	12.433	1.00	10.72
ATOM	721	CG	LEU	195	-10.918	15.321	12.860	1.00	10.49
ATOM	722	CD1	LEU	195	-10.531	16.104	14.087	1.00	11.81
ATOM	723	CD2	LEU	195	-10.812	13.826	13.122	1.00	12.25
ATOM	724	C	LEU	195	-14.234	15.121	10.836	1.00	9.94
ATOM	725	O	LEU	195	-14.995	14.225	11.197	1.00	11.31
ATOM	726	N	GLY	196	-14.653	16.206	10.192	1.00	9.82
ATOM	727	CA	GLY	196	-16.060	16.380	9.877	1.00	9.27
ATOM	728	C	GLY	196	-16.513	15.332	8.875	1.00	10.11
ATOM	729	O	GLY	196	-17.662	14.894	8.899	1.00	9.38
ATOM	730	N	GLN	197	-15.611	14.932	7.984	1.00	10.71
ATOM	731	CA	GLN	197	-15.925	13.920	6.981	1.00	13.11
ATOM	732	CB	GLN	197	-14.791	13.825	5.950	1.00	14.05
ATOM	733	CG	GLN	197	-14.671	15.026	5.013	1.00	17.85
ATOM	734	CD	GLN	197	-15.860	15.162	4.074	1.00	20.28
ATOM	735	OE1	GLN	197	-16.183	14.238	3.328	1.00	22.73
ATOM	736	NE2	GLN	197	-16.515	16.319	4.106	1.00	22.14
ATOM	737	C	GLN	197	-16.126	12.557	7.646	1.00	12.61
ATOM	738	O	GLN	197	-17.061	11.824	7.322	1.00	12.91
ATOM	739	N	ILE	198	-15.236	12.228	8.575	1.00	11.27
ATOM	740	CA	ILE	198	-15.287	10.958	9.288	1.00	10.19
ATOM	741	CB	ILE	198	-13.974	10.758	10.131	1.00	12.57
ATOM	742	CG2	ILE	198	-14.310	10.515	11.590	1.00	13.30
ATOM	743	CG1	ILE	198	-13.170	9.557	9.613	1.00	13.51
ATOM	744	CD1	ILE	198	-12.808	9.612	8.134	1.00	15.51
ATOM	745	C	ILE	198	-16.522	10.846	10.194	1.00	10.86
ATOM	746	O	ILE	198	-17.159	9.789	10.263	1.00	10.35
ATOM	747	N	PHE	199	-16.871	11.934	10.877	1.00	9.70
ATOM	748	CA	PHE	199	-18.011	11.906	11.790	1.00	12.37
ATOM	749	CB	PHE	199	-17.669	12.677	13.070	1.00	11.72
ATOM	750	CG	PHE	199	-16.508	12.099	13.834	1.00	11.17
ATOM	751	CD1	PHE	199	-15.319	12.804	13.953	1.00	11.14
ATOM	752	CD2	PHE	199	-16.603	10.842	14.430	1.00	13.46
ATOM	753	CE1	PHE	199	-14.235	12.272	14.655	1.00	11.35
ATOM	754	CE2	PHE	199	-15.520	10.297	15.136	1.00	11.84
ATOM	755	CZ	PHE	199	-14.336	11.017	15.248	1.00	13.15
ATOM	756	C	PHE	199	-19.356	12.397	11.248	1.00	13.95
ATOM	757	O	PHE	199	-20.402	12.050	11.801	1.00	14.66
ATOM	758	N	HIS	200	-19.343	13.191	10.179	1.00	13.73
ATOM	759	CA	HIS	200	-20.590	13.698	9.610	1.00	15.81
ATOM	760	CB	HIS	200	-20.497	15.201	9.324	1.00	15.90
ATOM	761	CG	HIS	200	-20.309	16.042	10.547	1.00	16.40
ATOM	762	CD2	HIS	200	-19.476	17.081	10.794	1.00	12.77
ATOM	763	ND1	HIS	200	-21.042	15.855	11.701	1.00	15.22
ATOM	764	CE1	HIS	200	-20.666	16.740	12.607	1.00	14.74
ATOM	765	NE2	HIS	200	-19.717	17.496	12.082	1.00	16.55

ATOM	766	C	HIS	200	-20.975	12.984	8.325	1.00	17.96
ATOM	767	O	HIS	200	-22.143	12.674	8.105	1.00	19.80
ATOM	768	N	ASN	201	-19.992	12.731	7.469	1.00	18.43
ATOM	769	CA	ASN	201	-20.254	12.064	6.206	1.00	19.28
ATOM	770	CB	ASN	201	-19.248	12.538	5.159	1.00	20.80
ATOM	771	CG	ASN	201	-19.351	14.028	4.900	1.00	24.90
ATOM	772	OD1	ASN	201	-20.312	14.498	4.291	1.00	26.82
ATOM	773	ND2	ASN	201	-18.369	14.782	5.377	1.00	28.11
ATOM	774	C	ASN	201	-20.215	10.549	6.352	1.00	19.08
ATOM	775	O	ASN	201	-21.233	9.883	6.151	1.00	19.44
ATOM	776	N	PHE	202	-19.057	9.995	6.703	1.00	16.90
ATOM	777	CA	PHE	202	-18.962	8.551	6.870	1.00	16.56
ATOM	778	CB	PHE	202	-17.502	8.110	7.005	1.00	17.57
ATOM	779	CG	PHE	202	-16.683	8.333	5.760	1.00	17.87
ATOM	780	CD1	PHE	202	-16.009	9.532	5.557	1.00	17.51
ATOM	781	CD2	PHE	202	-16.593	7.343	4.785	1.00	18.96
ATOM	782	CE1	PHE	202	-15.254	9.745	4.402	1.00	17.20
ATOM	783	CE2	PHE	202	-15.840	7.545	3.626	1.00	18.56
ATOM	784	CZ	PHE	202	-15.170	8.750	3.436	1.00	16.98
ATOM	785	C	PHE	202	-19.761	8.112	8.092	1.00	16.65
ATOM	786	O	PHE	202	-20.237	6.977	8.157	1.00	15.04
ATOM	787	N	ASN	203	-19.899	9.018	9.056	1.00	14.40
ATOM	788	CA	ASN	203	-20.661	8.766	10.277	1.00	16.92
ATOM	789	CB	ASN	203	-22.119	8.448	9.917	1.00	20.29
ATOM	790	CG	ASN	203	-23.052	8.525	11.116	1.00	25.21
ATOM	791	OD1	ASN	203	-24.171	8.010	11.075	1.00	28.86
ATOM	792	ND2	ASN	203	-22.604	9.180	12.185	1.00	24.70
ATOM	793	C	ASN	203	-20.092	7.649	11.157	1.00	15.74
ATOM	794	O	ASN	203	-20.824	6.769	11.610	1.00	16.18
ATOM	795	N	TYR	204	-18.786	7.690	11.400	1.00	15.51
ATOM	796	CA	TYR	204	-18.128	6.693	12.239	1.00	14.68
ATOM	797	CB	TYR	204	-16.647	6.589	11.873	1.00	16.02
ATOM	798	CG	TYR	204	-16.387	5.882	10.561	1.00	16.25
ATOM	799	CD1	TYR	204	-15.744	6.533	9.506	1.00	17.07
ATOM	800	CE1	TYR	204	-15.480	5.871	8.305	1.00	17.11
ATOM	801	CD2	TYR	204	-16.763	4.552	10.381	1.00	18.20
ATOM	802	CE2	TYR	204	-16.506	3.883	9.184	1.00	17.81
ATOM	803	CZ	TYR	204	-15.865	4.544	8.155	1.00	17.83
ATOM	804	OH	TYR	204	-15.602	3.873	6.983	1.00	21.39
ATOM	805	C	TYR	204	-18.280	7.078	13.708	1.00	14.27
ATOM	806	O	TYR	204	-18.361	8.258	14.039	1.00	13.49
ATOM	807	N	PRO	205	-18.305	6.082	14.611	1.00	13.73
ATOM	808	CD	PRO	205	-18.184	4.637	14.334	1.00	13.34
ATOM	809	CA	PRO	205	-18.454	6.318	16.050	1.00	13.07
ATOM	810	CB	PRO	205	-18.887	4.958	16.563	1.00	11.62
ATOM	811	CG	PRO	205	-18.044	4.042	15.736	1.00	12.91
ATOM	812	C	PRO	205	-17.185	6.809	16.740	1.00	11.56
ATOM	813	O	PRO	205	-17.227	7.273	17.878	1.00	9.98
ATOM	814	N	ALA	206	-16.060	6.695	16.044	1.00	11.21
ATOM	815	CA	ALA	206	-14.773	7.109	16.584	1.00	11.39
ATOM	816	CB	ALA	206	-14.364	6.172	17.725	1.00	11.56
ATOM	817	C	ALA	206	-13.745	7.058	15.460	1.00	11.75
ATOM	818	O	ALA	206	-14.068	6.652	14.340	1.00	13.80
ATOM	819	N	ALA	207	-12.514	7.477	15.749	1.00	12.60
ATOM	820	CA	ALA	207	-11.456	7.459	14.743	1.00	10.99
ATOM	821	CB	ALA	207	-11.706	8.555	13.717	1.00	12.04
ATOM	822	C	ALA	207	-10.049	7.611	15.325	1.00	12.35
ATOM	823	O	ALA	207	-9.844	8.261	16.356	1.00	10.59
ATOM	824	N	VAL	208	-9.077	6.996	14.659	1.00	12.20
ATOM	825	CA	VAL	208	-7.690	7.095	15.083	1.00	9.71
ATOM	826	CB	VAL	208	-6.993	5.711	15.098	1.00	12.11
ATOM	827	CG1	VAL	208	-5.498	5.873	15.391	1.00	7.06

ATOM	828	CG2	VAL	208	-7.637	4.820	16.167	1.00	9.13
ATOM	829	C	VAL	208	-7.006	8.019	14.079	1.00	10.15
ATOM	830	O	VAL	208	-6.876	7.688	12.899	1.00	9.92
ATOM	831	N	VAL	209	-6.591	9.186	14.562	1.00	8.96
ATOM	832	CA	VAL	209	-5.925	10.192	13.737	1.00	9.98
ATOM	833	CB	VAL	209	-6.094	11.611	14.342	1.00	10.09
ATOM	834	CG1	VAL	209	-5.540	12.652	13.384	1.00	8.08
ATOM	835	CG2	VAL	209	-7.562	11.888	14.649	1.00	8.06
ATOM	836	C	VAL	209	-4.428	9.887	13.640	1.00	11.61
ATOM	837	O	VAL	209	-3.738	9.799	14.659	1.00	11.51
ATOM	838	N	VAL	210	-3.933	9.749	12.413	1.00	11.00
ATOM	839	CA	VAL	210	-2.523	9.448	12.174	1.00	9.05
ATOM	840	CB	VAL	210	-2.338	7.994	11.689	1.00	10.36
ATOM	841	CG1	VAL	210	-0.859	7.703	11.489	1.00	10.36
ATOM	842	CG2	VAL	210	-2.957	7.025	12.688	1.00	9.58
ATOM	843	C	VAL	210	-1.932	10.367	11.111	1.00	9.17
ATOM	844	O	VAL	210	-2.363	10.351	9.961	1.00	7.52
ATOM	845	N	GLU	211	-0.941	11.167	11.483	1.00	7.86
ATOM	846	CA	GLU	211	-0.337	12.056	10.502	1.00	9.86
ATOM	847	CB	GLU	211	0.387	13.201	11.210	1.00	9.00
ATOM	848	CG	GLU	211	-0.567	13.977	12.113	1.00	12.94
ATOM	849	CD	GLU	211	0.030	15.243	12.673	1.00	13.59
ATOM	850	OE1	GLU	211	1.212	15.219	13.073	1.00	12.18
ATOM	851	OE2	GLU	211	-0.692	16.264	12.728	1.00	14.94
ATOM	852	C	GLU	211	0.591	11.268	9.572	1.00	9.98
ATOM	853	O	GLU	211	1.175	10.255	9.964	1.00	10.26
ATOM	854	N	ASP	212	0.705	11.743	8.336	1.00	9.36
ATOM	855	CA	ASP	212	1.504	11.095	7.300	1.00	9.55
ATOM	856	CB	ASP	212	1.443	11.927	6.017	1.00	10.09
ATOM	857	CG	ASP	212	2.106	13.279	6.175	1.00	9.44
ATOM	858	OD1	ASP	212	1.815	13.958	7.176	1.00	14.08
ATOM	859	OD2	ASP	212	2.913	13.665	5.306	1.00	14.14
ATOM	860	C	ASP	212	2.964	10.787	7.621	1.00	10.86
ATOM	861	O	ASP	212	3.584	9.975	6.928	1.00	10.80
ATOM	862	N	ASP	213	3.524	11.417	8.652	1.00	10.96
ATOM	863	CA	ASP	213	4.920	11.157	8.986	1.00	10.25
ATOM	864	CB	ASP	213	5.693	12.479	9.131	1.00	12.58
ATOM	865	CG	ASP	213	5.138	13.384	10.219	1.00	13.64
ATOM	866	OD1	ASP	213	4.050	13.092	10.761	1.00	10.84
ATOM	867	OD2	ASP	213	5.796	14.405	10.527	1.00	13.67
ATOM	868	C	ASP	213	5.109	10.274	10.218	1.00	9.70
ATOM	869	O	ASP	213	6.140	10.328	10.892	1.00	9.23
ATOM	870	N	LEU	214	4.115	9.436	10.496	1.00	8.23
ATOM	871	CA	LEU	214	4.198	8.533	11.636	1.00	8.07
ATOM	872	CB	LEU	214	3.014	8.734	12.589	1.00	8.64
ATOM	873	CG	LEU	214	2.720	10.137	13.132	1.00	10.35
ATOM	874	CD1	LEU	214	1.575	10.042	14.142	1.00	9.20
ATOM	875	CD2	LEU	214	3.964	10.725	13.787	1.00	7.22
ATOM	876	C	LEU	214	4.205	7.084	11.179	1.00	8.15
ATOM	877	O	LEU	214	3.444	6.696	10.285	1.00	9.56
ATOM	878	N	GLU	215	5.079	6.289	11.780	1.00	9.13
ATOM	879	CA	GLU	215	5.130	4.867	11.479	1.00	9.53
ATOM	880	CB	GLU	215	6.565	4.390	11.295	1.00	12.78
ATOM	881	CG	GLU	215	6.637	2.923	10.921	1.00	17.00
ATOM	882	CD	GLU	215	8.049	2.448	10.652	1.00	18.95
ATOM	883	OE1	GLU	215	8.783	3.150	9.924	1.00	19.11
ATOM	884	OE2	GLU	215	8.414	1.365	11.159	1.00	20.18
ATOM	885	C	GLU	215	4.516	4.173	12.691	1.00	10.18
ATOM	886	O	GLU	215	4.917	4.440	13.825	1.00	10.95
ATOM	887	N	VAL	216	3.545	3.295	12.457	1.00	9.36
ATOM	888	CA	VAL	216	2.886	2.584	13.550	1.00	9.56
ATOM	889	CB	VAL	216	1.431	2.210	13.177	1.00	9.32

ATOM	890	CG1	VAL	216	0.630	3.471	12.853	1.00	9.71
ATOM	891	CG2	VAL	216	1.427	1.256	11.989	1.00	9.80
ATOM	892	C	VAL	216	3.614	1.306	13.968	1.00	10.78
ATOM	893	O	VAL	216	4.298	0.668	13.163	1.00	9.99
ATOM	894	N	ALA	217	3.462	0.946	15.240	1.00	9.61
ATOM	895	CA	ALA	217	4.069	-0.260	15.794	1.00	9.85
ATOM	896	CB	ALA	217	4.144	-0.143	17.312	1.00	10.35
ATOM	897	C	ALA	217	3.217	-1.470	15.403	1.00	9.89
ATOM	898	O	ALA	217	2.060	-1.316	15.020	1.00	8.85
ATOM	899	N	PRO	218	3.777	-2.691	15.512	1.00	9.77
ATOM	900	CD	PRO	218	5.168	-2.972	15.919	1.00	11.12
ATOM	901	CA	PRO	218	3.073	-3.934	15.171	1.00	9.83
ATOM	902	CB	PRO	218	4.079	-5.019	15.568	1.00	8.57
ATOM	903	CG	PRO	218	5.405	-4.348	15.348	1.00	12.59
ATOM	904	C	PRO	218	1.737	-4.108	15.900	1.00	9.96
ATOM	905	O	PRO	218	0.782	-4.658	15.344	1.00	11.34
ATOM	906	N	ASP	219	1.679	-3.660	17.151	1.00	9.74
ATOM	907	CA	ASP	219	0.459	-3.785	17.935	1.00	10.53
ATOM	908	CB	ASP	219	0.778	-4.279	19.358	1.00	9.36
ATOM	909	CG	ASP	219	1.859	-3.458	20.047	1.00	10.55
ATOM	910	OD1	ASP	219	2.279	-2.418	19.501	1.00	9.50
ATOM	911	OD2	ASP	219	2.287	-3.856	21.152	1.00	11.02
ATOM	912	C	ASP	219	-0.324	-2.478	17.998	1.00	10.06
ATOM	913	O	ASP	219	-1.012	-2.202	18.974	1.00	10.64
ATOM	914	N	PHE	220	-0.219	-1.684	16.940	1.00	11.31
ATOM	915	CA	PHE	220	-0.917	-0.406	16.851	1.00	10.19
ATOM	916	CB	PHE	220	-0.553	0.281	15.531	1.00	11.57
ATOM	917	CG	PHE	220	-1.303	1.563	15.275	1.00	10.65
ATOM	918	CD1	PHE	220	-0.906	2.755	15.879	1.00	9.75
ATOM	919	CD2	PHE	220	-2.397	1.579	14.412	1.00	9.69
ATOM	920	CE1	PHE	220	-1.584	3.945	15.625	1.00	9.81
ATOM	921	CE2	PHE	220	-3.086	2.766	14.151	1.00	9.32
ATOM	922	CZ	PHE	220	-2.676	3.956	14.761	1.00	7.88
ATOM	923	C	PHE	220	-2.434	-0.581	16.936	1.00	10.17
ATOM	924	O	PHE	220	-3.089	0.051	17.763	1.00	10.38
ATOM	925	N	PHE	221	-2.987	-1.433	16.074	1.00	10.35
ATOM	926	CA	PHE	221	-4.426	-1.674	16.050	1.00	8.72
ATOM	927	CB	PHE	221	-4.815	-2.461	14.794	1.00	9.57
ATOM	928	CG	PHE	221	-4.330	-1.845	13.513	1.00	7.34
ATOM	929	CD1	PHE	221	-3.022	-2.058	13.072	1.00	6.84
ATOM	930	CD2	PHE	221	-5.178	-1.055	12.746	1.00	9.32
ATOM	931	CE1	PHE	221	-2.569	-1.489	11.877	1.00	7.86
ATOM	932	CE2	PHE	221	-4.739	-0.481	11.550	1.00	7.78
ATOM	933	CZ	PHE	221	-3.429	-0.701	11.116	1.00	8.58
ATOM	934	C	PHE	221	-4.882	-2.437	17.289	1.00	9.36
ATOM	935	O	PHE	221	-5.894	-2.095	17.904	1.00	9.88
ATOM	936	N	GLU	222	-4.137	-3.482	17.638	1.00	9.42
ATOM	937	CA	GLU	222	-4.429	-4.293	18.812	1.00	8.92
ATOM	938	CB	GLU	222	-3.246	-5.241	19.069	1.00	7.82
ATOM	939	CG	GLU	222	-3.340	-6.110	20.303	1.00	9.24
ATOM	940	CD	GLU	222	-4.412	-7.179	20.210	1.00	10.30
ATOM	941	OE1	GLU	222	-4.770	-7.586	19.084	1.00	8.81
ATOM	942	OE2	GLU	222	-4.880	-7.632	21.271	1.00	9.42
ATOM	943	C	GLU	222	-4.618	-3.340	19.990	1.00	8.96
ATOM	944	O	GLU	222	-5.581	-3.438	20.748	1.00	9.26
ATOM	945	N	TYR	223	-3.694	-2.396	20.112	1.00	7.87
ATOM	946	CA	TYR	223	-3.720	-1.411	21.181	1.00	9.38
ATOM	947	CB	TYR	223	-2.536	-0.462	21.002	1.00	8.05
ATOM	948	CG	TYR	223	-2.510	0.723	21.940	1.00	11.24
ATOM	949	CD1	TYR	223	-2.514	0.546	23.322	1.00	10.78
ATOM	950	CE1	TYR	223	-2.422	1.640	24.188	1.00	11.78
ATOM	951	CD2	TYR	223	-2.423	2.023	21.441	1.00	11.42

ATOM	952	CE2	TYR	223	-2.333	3.123	22.298	1.00	10.82
ATOM	953	CZ	TYR	223	-2.330	2.920	23.668	1.00	11.42
ATOM	954	OH	TYR	223	-2.209	3.994	24.518	1.00	9.77
ATOM	955	C	TYR	223	-5.033	-0.627	21.221	1.00	8.33
ATOM	956	O	TYR	223	-5.688	-0.542	22.263	1.00	7.32
ATOM	957	N	PHE	224	-5.430	-0.067	20.084	1.00	8.05
ATOM	958	CA	PHE	224	-6.659	0.708	20.042	1.00	9.80
ATOM	959	CB	PHE	224	-6.676	1.588	18.788	1.00	8.42
ATOM	960	CG	PHE	224	-5.693	2.722	18.849	1.00	8.78
ATOM	961	CD1	PHE	224	-4.491	2.665	18.153	1.00	7.69
ATOM	962	CD2	PHE	224	-5.948	3.825	19.659	1.00	8.38
ATOM	963	CE1	PHE	224	-3.550	3.695	18.264	1.00	8.78
ATOM	964	CE2	PHE	224	-5.020	4.854	19.778	1.00	9.06
ATOM	965	CZ	PHE	224	-3.816	4.789	19.078	1.00	8.73
ATOM	966	C	PHE	224	-7.956	-0.097	20.156	1.00	11.07
ATOM	967	O	PHE	224	-8.941	0.411	20.693	1.00	11.95
ATOM	968	N	GLN	225	-7.977	-1.336	19.666	1.00	12.62
ATOM	969	CA	GLN	225	-9.200	-2.136	19.783	1.00	12.79
ATOM	970	CB	GLN	225	-9.141	-3.381	18.888	1.00	16.61
ATOM	971	CG	GLN	225	-10.386	-4.294	18.949	1.00	19.76
ATOM	972	CD	GLN	225	-11.709	-3.576	18.643	1.00	25.30
ATOM	973	OE1	GLN	225	-12.321	-2.958	19.526	1.00	27.07
ATOM	974	NE2	GLN	225	-12.148	-3.652	17.387	1.00	24.87
ATOM	975	C	GLN	225	-9.391	-2.547	21.240	1.00	11.53
ATOM	976	O	GLN	225	-10.508	-2.777	21.689	1.00	11.00
ATOM	977	N	ALA	226	-8.295	-2.633	21.985	1.00	12.90
ATOM	978	CA	ALA	226	-8.383	-3.009	23.390	1.00	12.55
ATOM	979	CB	ALA	226	-7.065	-3.633	23.853	1.00	11.14
ATOM	980	C	ALA	226	-8.748	-1.823	24.286	1.00	12.68
ATOM	981	O	ALA	226	-9.459	-1.991	25.280	1.00	11.99
ATOM	982	N	THR	227	-8.274	-0.628	23.937	1.00	11.59
ATOM	983	CA	THR	227	-8.554	0.554	24.744	1.00	11.61
ATOM	984	CB	THR	227	-7.364	1.559	24.725	1.00	12.03
ATOM	985	OG1	THR	227	-7.081	1.965	23.377	1.00	10.25
ATOM	986	CG2	THR	227	-6.117	0.920	25.341	1.00	10.96
ATOM	987	C	THR	227	-9.832	1.301	24.360	1.00	12.33
ATOM	988	O	THR	227	-10.304	2.156	25.114	1.00	10.90
ATOM	989	N	TYR	228	-10.397	0.983	23.200	1.00	12.36
ATOM	990	CA	TYR	228	-11.625	1.643	22.763	1.00	14.48
ATOM	991	CB	TYR	228	-12.061	1.088	21.403	1.00	16.98
ATOM	992	CG	TYR	228	-13.403	1.590	20.924	1.00	19.03
ATOM	993	CD1	TYR	228	-13.639	2.952	20.743	1.00	20.29
ATOM	994	CE1	TYR	228	-14.874	3.418	20.290	1.00	19.90
ATOM	995	CD2	TYR	228	-14.438	0.697	20.640	1.00	20.69
ATOM	996	CE2	TYR	228	-15.675	1.148	20.186	1.00	22.12
ATOM	997	CZ	TYR	228	-15.885	2.508	20.015	1.00	21.24
ATOM	998	OH	TYR	228	-17.102	2.955	19.564	1.00	22.46
ATOM	999	C	TYR	228	-12.755	1.479	23.794	1.00	13.65
ATOM	1000	O	TYR	228	-13.446	2.443	24.126	1.00	11.80
ATOM	1001	N	PRO	229	-12.957	0.255	24.313	1.00	14.20
ATOM	1002	CD	PRO	229	-12.310	-1.018	23.946	1.00	15.24
ATOM	1003	CA	PRO	229	-14.017	0.032	25.304	1.00	14.21
ATOM	1004	CB	PRO	229	-13.898	-1.459	25.614	1.00	16.20
ATOM	1005	CG	PRO	229	-13.368	-2.033	24.327	1.00	17.48
ATOM	1006	C	PRO	229	-13.832	0.882	26.559	1.00	13.69
ATOM	1007	O	PRO	229	-14.809	1.298	27.185	1.00	13.42
ATOM	1008	N	LEU	230	-12.577	1.125	26.929	1.00	12.63
ATOM	1009	CA	LEU	230	-12.279	1.922	28.111	1.00	14.29
ATOM	1010	CB	LEU	230	-10.794	1.825	28.464	1.00	15.70
ATOM	1011	CG	LEU	230	-10.390	1.140	29.768	1.00	20.66
ATOM	1012	CD1	LEU	230	-8.918	1.421	30.016	1.00	22.16
ATOM	1013	CD2	LEU	230	-11.221	1.658	30.933	1.00	20.53

ATOM	1014	C	LEU	230	-12.647	3.382	27.872	1.00	13.73
ATOM	1015	O	LEU	230	-13.172	4.053	28.759	1.00	12.84
ATOM	1016	N	LEU	231	-12.370	3.868	26.669	1.00	15.44
ATOM	1017	CA	LEU	231	-12.678	5.251	26.329	1.00	17.38
ATOM	1018	CB	LEU	231	-12.113	5.602	24.948	1.00	14.30
ATOM	1019	CG	LEU	231	-12.271	7.067	24.540	1.00	14.94
ATOM	1020	CD1	LEU	231	-11.688	7.967	25.622	1.00	10.96
ATOM	1021	CD2	LEU	231	-11.583	7.308	23.200	1.00	12.85
ATOM	1022	C	LEU	231	-14.187	5.479	26.347	1.00	18.16
ATOM	1023	O	LEU	231	-14.659	6.544	26.747	1.00	18.93
ATOM	1024	N	LYS	232	-14.943	4.473	25.923	1.00	19.40
ATOM	1025	CA	LYS	232	-16.398	4.588	25.905	1.00	21.69
ATOM	1026	CB	LYS	232	-17.018	3.526	24.993	1.00	23.79
ATOM	1027	CG	LYS	232	-17.199	3.954	23.548	1.00	26.37
ATOM	1028	CD	LYS	232	-18.342	3.188	22.896	1.00	30.83
ATOM	1029	CE	LYS	232	-18.108	1.680	22.929	1.00	33.09
ATOM	1030	NZ	LYS	232	-19.259	0.919	22.354	1.00	34.64
ATOM	1031	C	LYS	232	-17.032	4.467	27.285	1.00	21.54
ATOM	1032	O	LYS	232	-18.095	5.039	27.532	1.00	22.02
ATOM	1033	N	ALA	233	-16.378	3.735	28.184	1.00	19.81
ATOM	1034	CA	ALA	233	-16.917	3.516	29.524	1.00	20.08
ATOM	1035	CB	ALA	233	-16.597	2.093	29.979	1.00	19.67
ATOM	1036	C	ALA	233	-16.475	4.500	30.597	1.00	19.79
ATOM	1037	O	ALA	233	-17.100	4.585	31.657	1.00	22.27
ATOM	1038	N	ASP	234	-15.406	5.242	30.339	1.00	17.49
ATOM	1039	CA	ASP	234	-14.907	6.190	31.325	1.00	15.11
ATOM	1040	CB	ASP	234	-13.507	5.759	31.765	1.00	15.98
ATOM	1041	CG	ASP	234	-12.981	6.568	32.925	1.00	13.13
ATOM	1042	OD1	ASP	234	-13.624	7.570	33.314	1.00	13.23
ATOM	1043	OD2	ASP	234	-11.909	6.199	33.447	1.00	15.87
ATOM	1044	C	ASP	234	-14.873	7.611	30.754	1.00	15.82
ATOM	1045	O	ASP	234	-13.954	7.971	30.020	1.00	14.78
ATOM	1046	N	PRO	235	-15.884	8.433	31.088	1.00	14.94
ATOM	1047	CD	PRO	235	-17.034	8.076	31.939	1.00	14.58
ATOM	1048	CA	PRO	235	-15.998	9.820	30.622	1.00	14.07
ATOM	1049	CB	PRO	235	-17.389	10.232	31.102	1.00	12.91
ATOM	1050	CG	PRO	235	-17.553	9.435	32.361	1.00	13.89
ATOM	1051	C	PRO	235	-14.902	10.753	31.125	1.00	13.75
ATOM	1052	O	PRO	235	-14.778	11.883	30.646	1.00	15.16
ATOM	1053	N	SER	236	-14.113	10.294	32.094	1.00	12.24
ATOM	1054	CA	SER	236	-13.020	11.118	32.605	1.00	9.22
ATOM	1055	CB	SER	236	-12.621	10.684	34.025	1.00	7.71
ATOM	1056	OG	SER	236	-12.008	9.409	34.037	1.00	10.86
ATOM	1057	C	SER	236	-11.840	10.972	31.635	1.00	8.91
ATOM	1058	O	SER	236	-10.818	11.648	31.763	1.00	8.62
ATOM	1059	N	LEU	237	-11.997	10.075	30.666	1.00	8.56
ATOM	1060	CA	LEU	237	-10.987	9.856	29.631	1.00	10.42
ATOM	1061	CB	LEU	237	-10.796	8.361	29.353	1.00	8.06
ATOM	1062	CG	LEU	237	-10.027	7.469	30.331	1.00	10.68
ATOM	1063	CD1	LEU	237	-10.054	6.028	29.825	1.00	10.17
ATOM	1064	CD2	LEU	237	-8.593	7.969	30.463	1.00	10.21
ATOM	1065	C	LEU	237	-11.527	10.508	28.365	1.00	10.40
ATOM	1066	O	LEU	237	-12.709	10.354	28.046	1.00	10.59
ATOM	1067	N	TRP	238	-10.691	11.240	27.637	1.00	12.27
ATOM	1068	CA	TRP	238	-11.178	11.854	26.409	1.00	10.08
ATOM	1069	CB	TRP	238	-11.261	13.383	26.567	1.00	11.06
ATOM	1070	CG	TRP	238	-9.968	14.145	26.498	1.00	12.03
ATOM	1071	CD2	TRP	238	-9.798	15.486	26.017	1.00	12.07
ATOM	1072	CE2	TRP	238	-8.434	15.817	26.173	1.00	13.11
ATOM	1073	CE3	TRP	238	-10.668	16.439	25.472	1.00	12.20
ATOM	1074	CD1	TRP	238	-8.737	13.729	26.915	1.00	12.58
ATOM	1075	NE1	TRP	238	-7.808	14.729	26.721	1.00	14.70

ATOM	1076	CZ2	TRP	238	-7.918	17.063	25.800	1.00	13.84
ATOM	1077	CZ3	TRP	238	-10.155	17.678	25.100	1.00	13.81
ATOM	1078	CH2	TRP	238	-8.792	17.977	25.266	1.00	13.91
ATOM	1079	C	TRP	238	-10.342	11.446	25.198	1.00	10.46
ATOM	1080	O	TRP	238	-10.572	11.912	24.082	1.00	9.14
ATOM	1081	N	CYS	239	-9.388	10.543	25.418	1.00	9.67
ATOM	1082	CA	CYS	239	-8.547	10.065	24.327	1.00	11.07
ATOM	1083	C	CYS	239	-7.610	8.926	24.697	1.00	10.15
ATOM	1084	O	CYS	239	-7.364	8.658	25.872	1.00	9.42
ATOM	1085	CB	CYS	239	-7.753	11.242	23.749	1.00	14.26
ATOM	1086	SG	CYS	239	-5.928	11.266	23.856	1.00	14.33
ATOM	1087	N	VAL	240	-7.128	8.233	23.671	1.00	9.22
ATOM	1088	CA	VAL	240	-6.175	7.145	23.832	1.00	9.18
ATOM	1089	CB	VAL	240	-6.796	5.765	23.508	1.00	8.62
ATOM	1090	CG1	VAL	240	-5.724	4.667	23.615	1.00	6.40
ATOM	1091	CG2	VAL	240	-7.940	5.470	24.482	1.00	7.72
ATOM	1092	C	VAL	240	-5.069	7.460	22.835	1.00	9.53
ATOM	1093	O	VAL	240	-5.299	7.495	21.622	1.00	10.50
ATOM	1094	N	SER	241	-3.871	7.711	23.351	1.00	10.64
ATOM	1095	CA	SER	241	-2.740	8.054	22.502	1.00	9.53
ATOM	1096	CB	SER	241	-2.131	9.384	22.962	1.00	9.78
ATOM	1097	OG	SER	241	-1.001	9.720	22.175	1.00	9.36
ATOM	1098	C	SER	241	-1.668	6.971	22.494	1.00	9.44
ATOM	1099	O	SER	241	-1.464	6.268	23.483	1.00	8.63
ATOM	1100	N	ALA	242	-0.994	6.839	21.358	1.00	9.47
ATOM	1101	CA	ALA	242	0.066	5.853	21.192	1.00	8.39
ATOM	1102	CB	ALA	242	0.150	5.441	19.727	1.00	7.59
ATOM	1103	C	ALA	242	1.405	6.441	21.622	1.00	8.94
ATOM	1104	O	ALA	242	2.407	5.731	21.713	1.00	11.04
ATOM	1105	N	TRP	243	1.402	7.734	21.921	1.00	8.55
ATOM	1106	CA	TRP	243	2.627	8.455	22.245	1.00	9.18
ATOM	1107	CB	TRP	243	2.567	9.809	21.523	1.00	8.70
ATOM	1108	CG	TRP	243	3.866	10.556	21.414	1.00	10.47
ATOM	1109	CD2	TRP	243	4.834	10.436	20.363	1.00	12.47
ATOM	1110	CE2	TRP	243	5.876	11.347	20.645	1.00	13.27
ATOM	1111	CE3	TRP	243	4.921	9.645	19.209	1.00	10.51
ATOM	1112	CD1	TRP	243	4.348	11.506	22.271	1.00	13.44
ATOM	1113	NE1	TRP	243	5.557	11.989	21.814	1.00	13.13
ATOM	1114	CZ2	TRP	243	6.992	11.491	19.813	1.00	14.30
ATOM	1115	CZ3	TRP	243	6.035	9.790	18.378	1.00	12.49
ATOM	1116	CH2	TRP	243	7.054	10.707	18.689	1.00	12.47
ATOM	1117	C	TRP	243	3.028	8.674	23.704	1.00	10.61
ATOM	1118	O	TRP	243	2.228	9.110	24.537	1.00	10.98
ATOM	1119	N	ASN	244	4.286	8.356	24.000	1.00	8.65
ATOM	1120	CA	ASN	244	4.845	8.586	25.328	1.00	9.62
ATOM	1121	CB	ASN	244	5.614	7.362	25.844	1.00	8.73
ATOM	1122	CG	ASN	244	6.338	7.646	27.156	1.00	11.29
ATOM	1123	OD1	ASN	244	6.269	8.760	27.678	1.00	11.54
ATOM	1124	ND2	ASN	244	7.035	6.648	27.690	1.00	9.17
ATOM	1125	C	ASN	244	5.815	9.742	25.095	1.00	9.49
ATOM	1126	O	ASN	244	6.842	9.568	24.438	1.00	8.91
ATOM	1127	N	ASP	245	5.483	10.921	25.613	1.00	9.62
ATOM	1128	CA	ASP	245	6.320	12.107	25.420	1.00	11.51
ATOM	1129	CB	ASP	245	5.665	13.311	26.098	1.00	11.16
ATOM	1130	CG	ASP	245	4.482	13.838	25.309	1.00	14.28
ATOM	1131	OD1	ASP	245	4.707	14.497	24.272	1.00	12.68
ATOM	1132	OD2	ASP	245	3.327	13.582	25.711	1.00	14.86
ATOM	1133	C	ASP	245	7.770	11.970	25.876	1.00	12.01
ATOM	1134	O	ASP	245	8.653	12.668	25.370	1.00	11.09
ATOM	1135	N	ASN	246	8.014	11.079	26.832	1.00	13.09
ATOM	1136	CA	ASN	246	9.362	10.844	27.336	1.00	13.22
ATOM	1137	CB	ASN	246	9.395	11.046	28.854	1.00	14.73

ATOM	1138	CG	ASN	246	9.073	12.472	29.259	1.00	15.20
ATOM	1139	OD1	ASN	246	9.785	13.411	28.891	1.00	17.35
ATOM	1140	ND2	ASN	246	7.992	12.646	30.015	1.00	13.37
ATOM	1141	C	ASN	246	9.787	9.417	26.991	1.00	14.77
ATOM	1142	O	ASN	246	10.606	8.813	27.685	1.00	15.26
ATOM	1143	N	GLY	247	9.235	8.893	25.899	1.00	14.52
ATOM	1144	CA	GLY	247	9.531	7.532	25.487	1.00	14.77
ATOM	1145	C	GLY	247	10.852	7.241	24.791	1.00	15.65
ATOM	1146	O	GLY	247	10.877	6.477	23.822	1.00	14.95
ATOM	1147	N	LYS	248	11.943	7.838	25.262	1.00	14.97
ATOM	1148	CA	LYS	248	13.254	7.584	24.672	1.00	16.08
ATOM	1149	CB	LYS	248	14.278	8.606	25.173	1.00	19.13
ATOM	1150	CG	LYS	248	13.937	10.054	24.842	1.00	21.46
ATOM	1151	CD	LYS	248	15.020	10.983	25.364	1.00	25.19
ATOM	1152	CE	LYS	248	14.706	12.440	25.080	1.00	26.85
ATOM	1153	NZ	LYS	248	15.773	13.334	25.630	1.00	27.05
ATOM	1154	C	LYS	248	13.673	6.172	25.086	1.00	16.40
ATOM	1155	O	LYS	248	13.192	5.653	26.096	1.00	15.23
ATOM	1156	N	GLU	249	14.569	5.553	24.322	1.00	16.00
ATOM	1157	CA	GLU	249	14.997	4.186	24.615	1.00	15.41
ATOM	1158	CB	GLU	249	16.069	3.727	23.615	1.00	18.34
ATOM	1159	CG	GLU	249	16.509	2.267	23.814	1.00	22.98
ATOM	1160	CD	GLU	249	17.575	1.819	22.819	1.00	26.80
ATOM	1161	OE1	GLU	249	17.250	1.636	21.625	1.00	29.86
ATOM	1162	OE2	GLU	249	18.744	1.653	23.229	1.00	28.06
ATOM	1163	C	GLU	249	15.491	3.917	26.038	1.00	13.39
ATOM	1164	O	GLU	249	15.055	2.959	26.665	1.00	13.31
ATOM	1165	N	GLN	250	16.395	4.743	26.552	1.00	12.33
ATOM	1166	CA	GLN	250	16.915	4.520	27.898	1.00	13.18
ATOM	1167	CB	GLN	250	18.286	5.188	28.066	1.00	14.91
ATOM	1168	CG	GLN	250	19.385	4.624	27.167	1.00	17.61
ATOM	1169	CD	GLN	250	19.551	3.117	27.299	1.00	18.41
ATOM	1170	OE1	GLN	250	19.751	2.591	28.398	1.00	20.30
ATOM	1171	NE2	GLN	250	19.473	2.414	26.173	1.00	20.44
ATOM	1172	C	GLN	250	15.977	5.004	29.001	1.00	12.32
ATOM	1173	O	GLN	250	16.313	4.920	30.183	1.00	11.54
ATOM	1174	N	MET	251	14.801	5.494	28.621	1.00	11.41
ATOM	1175	CA	MET	251	13.846	5.986	29.603	1.00	11.72
ATOM	1176	CB	MET	251	13.522	7.452	29.322	1.00	12.06
ATOM	1177	CG	MET	251	14.704	8.377	29.612	1.00	14.62
ATOM	1178	SD	MET	251	14.346	10.103	29.330	1.00	21.18
ATOM	1179	CE	MET	251	13.611	10.534	30.882	1.00	16.99
ATOM	1180	C	MET	251	12.561	5.176	29.706	1.00	11.91
ATOM	1181	O	MET	251	11.613	5.597	30.370	1.00	9.95
ATOM	1182	N	VAL	252	12.527	4.022	29.043	1.00	11.43
ATOM	1183	CA	VAL	252	11.360	3.145	29.093	1.00	9.88
ATOM	1184	CB	VAL	252	10.600	3.092	27.736	1.00	7.78
ATOM	1185	CG1	VAL	252	10.191	4.497	27.308	1.00	9.43
ATOM	1186	CG2	VAL	252	11.466	2.439	26.665	1.00	7.99
ATOM	1187	C	VAL	252	11.824	1.737	29.457	1.00	12.75
ATOM	1188	O	VAL	252	12.959	1.348	29.147	1.00	11.67
ATOM	1189	N	ASP	253	10.944	0.988	30.120	1.00	11.19
ATOM	1190	CA	ASP	253	11.216	-0.385	30.553	1.00	12.18
ATOM	1191	CB	ASP	253	10.414	-0.691	31.824	1.00	12.11
ATOM	1192	CG	ASP	253	10.773	-2.031	32.445	1.00	12.04
ATOM	1193	OD1	ASP	253	11.335	-2.904	31.745	1.00	11.95
ATOM	1194	OD2	ASP	253	10.475	-2.217	33.644	1.00	11.44
ATOM	1195	C	ASP	253	10.808	-1.354	29.444	1.00	13.74
ATOM	1196	O	ASP	253	9.621	-1.654	29.270	1.00	14.80
ATOM	1197	N	SER	254	11.791	-1.854	28.701	1.00	13.69
ATOM	1198	CA	SER	254	11.510	-2.768	27.600	1.00	14.87
ATOM	1199	CB	SER	254	12.785	-3.020	26.787	1.00	15.91

ATOM	1200	OG	SER	254	13.812	-3.553	27.606	1.00	20.40
ATOM	1201	C	SER	254	10.903	-4.098	28.033	1.00	13.97
ATOM	1202	O	SER	254	10.438	-4.864	27.189	1.00	12.85
ATOM	1203	N	SER	255	10.903	-4.376	29.336	1.00	12.45
ATOM	1204	CA	SER	255	10.337	-5.627	29.836	1.00	11.56
ATOM	1205	CB	SER	255	11.121	-6.139	31.052	1.00	10.01
ATOM	1206	OG	SER	255	10.830	-5.388	32.220	1.00	10.74
ATOM	1207	C	SER	255	8.866	-5.460	30.207	1.00	12.10
ATOM	1208	O	SER	255	8.225	-6.403	30.677	1.00	12.32
ATOM	1209	N	LYS	256	8.336	-4.256	30.004	1.00	10.71
ATOM	1210	CA	LYS	256	6.926	-3.980	30.284	1.00	9.05
ATOM	1211	CB	LYS	256	6.773	-3.095	31.527	1.00	9.64
ATOM	1212	CG	LYS	256	7.129	-3.776	32.853	1.00	11.19
ATOM	1213	CD	LYS	256	6.241	-4.990	33.150	1.00	13.94
ATOM	1214	CE	LYS	256	4.844	-4.606	33.652	1.00	13.82
ATOM	1215	NZ	LYS	256	4.126	-3.711	32.713	1.00	22.82
ATOM	1216	C	LYS	256	6.302	-3.271	29.084	1.00	8.64
ATOM	1217	O	LYS	256	5.743	-2.189	29.222	1.00	6.53
ATOM	1218	N	PRO	257	6.382	-3.874	27.888	1.00	7.56
ATOM	1219	CD	PRO	257	6.891	-5.207	27.508	1.00	7.07
ATOM	1220	CA	PRO	257	5.784	-3.187	26.739	1.00	6.92
ATOM	1221	CB	PRO	257	6.257	-4.024	25.560	1.00	6.73
ATOM	1222	CG	PRO	257	6.253	-5.430	26.143	1.00	7.05
ATOM	1223	C	PRO	257	4.260	-3.105	26.835	1.00	8.28
ATOM	1224	O	PRO	257	3.613	-2.384	26.068	1.00	8.69
ATOM	1225	N	GLU	258	3.696	-3.825	27.799	1.00	7.57
ATOM	1226	CA	GLU	258	2.252	-3.861	27.993	1.00	6.89
ATOM	1227	CB	GLU	258	1.842	-5.226	28.554	1.00	10.25
ATOM	1228	CG	GLU	258	2.195	-5.390	30.035	1.00	11.29
ATOM	1229	CD	GLU	258	3.514	-6.100	30.279	1.00	13.65
ATOM	1230	OE1	GLU	258	4.432	-5.967	29.447	1.00	13.04
ATOM	1231	OE2	GLU	258	3.636	-6.779	31.318	1.00	13.00
ATOM	1232	C	GLU	258	1.753	-2.783	28.954	1.00	8.96
ATOM	1233	O	GLU	258	0.563	-2.467	28.978	1.00	8.88
ATOM	1234	N	LEU	259	2.658	-2.232	29.755	1.00	7.99
ATOM	1235	CA	LEU	259	2.287	-1.223	30.747	1.00	7.39
ATOM	1236	CB	LEU	259	3.496	-0.883	31.620	1.00	6.09
ATOM	1237	CG	LEU	259	3.221	0.075	32.782	1.00	8.30
ATOM	1238	CD1	LEU	259	2.109	-0.477	33.657	1.00	7.33
ATOM	1239	CD2	LEU	259	4.492	0.272	33.582	1.00	9.48
ATOM	1240	C	LEU	259	1.696	0.062	30.172	1.00	6.86
ATOM	1241	O	LEU	259	2.285	0.693	29.300	1.00	8.36
ATOM	1242	N	LEU	260	0.526	0.447	30.674	1.00	7.17
ATOM	1243	CA	LEU	260	-0.139	1.666	30.217	1.00	9.19
ATOM	1244	CB	LEU	260	-1.499	1.337	29.594	1.00	9.21
ATOM	1245	CG	LEU	260	-1.465	0.333	28.446	1.00	7.29
ATOM	1246	CD1	LEU	260	-2.888	0.057	27.971	1.00	8.68
ATOM	1247	CD2	LEU	260	-0.609	0.883	27.310	1.00	8.92
ATOM	1248	C	LEU	260	-0.335	2.641	31.373	1.00	9.70
ATOM	1249	O	LEU	260	-0.245	2.254	32.542	1.00	10.81
ATOM	1250	N	TYR	261	-0.604	3.901	31.032	1.00	9.63
ATOM	1251	CA	TYR	261	-0.805	4.963	32.017	1.00	9.10
ATOM	1252	CB	TYR	261	0.456	5.824	32.160	1.00	8.08
ATOM	1253	CG	TYR	261	1.731	5.124	32.576	1.00	9.14
ATOM	1254	CD1	TYR	261	2.520	4.445	31.648	1.00	10.53
ATOM	1255	CE1	TYR	261	3.731	3.859	32.030	1.00	8.84
ATOM	1256	CD2	TYR	261	2.178	5.194	33.893	1.00	9.93
ATOM	1257	CE2	TYR	261	3.372	4.617	34.281	1.00	8.90
ATOM	1258	CZ	TYR	261	4.145	3.953	33.350	1.00	8.89
ATOM	1259	OH	TYR	261	5.330	3.386	33.754	1.00	8.63
ATOM	1260	C	TYR	261	-1.921	5.929	31.620	1.00	9.83
ATOM	1261	O	TYR	261	-2.455	5.877	30.510	1.00	10.36

ATOM	1262	N	ARG	262	-2.244	6.824	32.549	1.00	10.73
ATOM	1263	CA	ARG	262	-3.213	7.888	32.320	1.00	10.22
ATOM	1264	CB	ARG	262	-4.215	8.011	33.486	1.00	11.10
ATOM	1265	CG	ARG	262	-5.306	6.929	33.542	1.00	10.81
ATOM	1266	CD	ARG	262	-6.270	7.160	34.721	1.00	11.48
ATOM	1267	NE	ARG	262	-7.152	8.313	34.526	1.00	11.72
ATOM	1268	CZ	ARG	262	-8.427	8.227	34.148	1.00	11.14
ATOM	1269	NH1	ARG	262	-8.981	7.042	33.922	1.00	9.82
ATOM	1270	NH2	ARG	262	-9.154	9.326	33.994	1.00	13.10
ATOM	1271	C	ARG	262	-2.330	9.142	32.282	1.00	11.24
ATOM	1272	O	ARG	262	-1.304	9.193	32.972	1.00	10.45
ATOM	1273	N	THR	263	-2.697	10.127	31.464	1.00	10.03
ATOM	1274	CA	THR	263	-1.943	11.386	31.387	1.00	9.36
ATOM	1275	CB	THR	263	-0.877	11.380	30.260	1.00	8.67
ATOM	1276	OG1	THR	263	-0.197	12.644	30.252	1.00	8.19
ATOM	1277	CG2	THR	263	-1.521	11.167	28.903	1.00	5.38
ATOM	1278	C	THR	263	-2.853	12.589	31.145	1.00	10.88
ATOM	1279	O	THR	263	-3.785	12.525	30.341	1.00	11.53
ATOM	1280	N	ASP	264	-2.573	13.684	31.849	1.00	9.26
ATOM	1281	CA	ASP	264	-3.340	14.922	31.713	1.00	10.76
ATOM	1282	CB	ASP	264	-3.148	15.804	32.954	1.00	8.38
ATOM	1283	CG	ASP	264	-3.821	15.235	34.186	1.00	9.16
ATOM	1284	OD1	ASP	264	-3.197	15.253	35.272	1.00	10.22
ATOM	1285	OD2	ASP	264	-4.982	14.786	34.072	1.00	6.53
ATOM	1286	C	ASP	264	-2.860	15.680	30.479	1.00	10.63
ATOM	1287	O	ASP	264	-3.567	16.539	29.946	1.00	11.49
ATOM	1288	N	PHE	265	-1.654	15.347	30.027	1.00	10.47
ATOM	1289	CA	PHE	265	-1.044	15.986	28.866	1.00	9.64
ATOM	1290	CB	PHE	265	0.486	15.983	29.020	1.00	9.08
ATOM	1291	CG	PHE	265	1.202	16.905	28.064	1.00	10.03
ATOM	1292	CD1	PHE	265	1.571	18.184	28.458	1.00	9.48
ATOM	1293	CD2	PHE	265	1.510	16.490	26.766	1.00	9.58
ATOM	1294	CE1	PHE	265	2.236	19.038	27.580	1.00	8.80
ATOM	1295	CE2	PHE	265	2.173	17.337	25.882	1.00	6.69
ATOM	1296	CZ	PHE	265	2.537	18.609	26.286	1.00	8.22
ATOM	1297	C	PHE	265	-1.429	15.266	27.569	1.00	9.30
ATOM	1298	O	PHE	265	-1.016	14.120	27.335	1.00	7.44
ATOM	1299	N	PHE	266	-2.219	15.944	26.735	1.00	8.11
ATOM	1300	CA	PHE	266	-2.662	15.406	25.451	1.00	8.08
ATOM	1301	CB	PHE	266	-3.640	16.382	24.782	1.00	7.43
ATOM	1302	CG	PHE	266	-4.073	15.956	23.405	1.00	9.79
ATOM	1303	CD1	PHE	266	-4.814	14.790	23.225	1.00	10.59
ATOM	1304	CD2	PHE	266	-3.718	16.702	22.288	1.00	8.68
ATOM	1305	CE1	PHE	266	-5.195	14.373	21.952	1.00	11.51
ATOM	1306	CE2	PHE	266	-4.093	16.293	21.009	1.00	7.01
ATOM	1307	CZ	PHE	266	-4.834	15.127	20.840	1.00	9.44
ATOM	1308	C	PHE	266	-1.442	15.199	24.549	1.00	8.22
ATOM	1309	O	PHE	266	-0.771	16.169	24.166	1.00	9.39
ATOM	1310	N	PRO	267	-1.140	13.937	24.190	1.00	7.59
ATOM	1311	CD	PRO	267	-1.637	12.707	24.827	1.00	6.68
ATOM	1312	CA	PRO	267	0.016	13.628	23.334	1.00	6.91
ATOM	1313	CB	PRO	267	0.391	12.201	23.750	1.00	5.47
ATOM	1314	CG	PRO	267	-0.357	11.974	25.065	1.00	7.41
ATOM	1315	C	PRO	267	-0.216	13.700	21.828	1.00	6.53
ATOM	1316	O	PRO	267	0.707	13.995	21.073	1.00	6.50
ATOM	1317	N	GLY	268	-1.438	13.418	21.391	1.00	7.30
ATOM	1318	CA	GLY	268	-1.714	13.431	19.967	1.00	9.49
ATOM	1319	C	GLY	268	-0.862	12.333	19.357	1.00	9.93
ATOM	1320	O	GLY	268	-0.760	11.242	19.924	1.00	8.86
ATOM	1321	N	LEU	269	-0.252	12.619	18.209	1.00	9.09
ATOM	1322	CA	LEU	269	0.625	11.675	17.518	1.00	9.61
ATOM	1323	CB	LEU	269	2.034	11.775	18.114	1.00	9.40

ATOM	1324	CG	LEU	269	2.590	13.193	17.922	1.00	8.96
ATOM	1325	CD1	LEU	269	3.884	13.392	18.706	1.00	9.67
ATOM	1326	CD2	LEU	269	2.800	13.429	16.432	1.00	6.49
ATOM	1327	C	LEU	269	0.131	10.230	17.544	1.00	9.46
ATOM	1328	O	LEU	269	0.765	9.349	18.123	1.00	10.77
ATOM	1329	N	GLY	270	-0.990	9.993	16.870	1.00	9.13
ATOM	1330	CA	GLY	270	-1.583	8.670	16.845	1.00	8.95
ATOM	1331	C	GLY	270	-2.546	8.630	18.013	1.00	10.92
ATOM	1332	O	GLY	270	-2.212	8.121	19.082	1.00	9.86
ATOM	1333	N	TRP	271	-3.743	9.175	17.821	1.00	10.98
ATOM	1334	CA	TRP	271	-4.717	9.205	18.905	1.00	11.65
ATOM	1335	CB	TRP	271	-4.665	10.548	19.634	1.00	10.79
ATOM	1336	CG	TRP	271	-4.946	11.730	18.759	1.00	11.13
ATOM	1337	CD2	TRP	271	-6.097	12.582	18.811	1.00	9.33
ATOM	1338	CE2	TRP	271	-5.918	13.584	17.830	1.00	11.29
ATOM	1339	CE3	TRP	271	-7.260	12.598	19.593	1.00	10.93
ATOM	1340	CD1	TRP	271	-4.141	12.233	17.773	1.00	9.58
ATOM	1341	NE1	TRP	271	-4.718	13.347	17.213	1.00	9.54
ATOM	1342	CZ2	TRP	271	-6.862	14.597	17.609	1.00	8.85
ATOM	1343	CZ3	TRP	271	-8.199	13.604	19.375	1.00	10.76
ATOM	1344	CH2	TRP	271	-7.990	14.592	18.387	1.00	11.31
ATOM	1345	C	TRP	271	-6.145	8.930	18.487	1.00	11.67
ATOM	1346	O	TRP	271	-6.585	9.324	17.403	1.00	12.18
ATOM	1347	N	LEU	272	-6.860	8.260	19.383	1.00	10.89
ATOM	1348	CA	LEU	272	-8.252	7.889	19.189	1.00	11.38
ATOM	1349	CB	LEU	272	-8.471	6.472	19.728	1.00	10.82
ATOM	1350	CG	LEU	272	-9.904	5.967	19.917	1.00	11.62
ATOM	1351	CD1	LEU	272	-10.510	5.583	18.572	1.00	8.90
ATOM	1352	CD2	LEU	272	-9.886	4.768	20.857	1.00	9.42
ATOM	1353	C	LEU	272	-9.200	8.849	19.913	1.00	10.82
ATOM	1354	O	LEU	272	-8.964	9.226	21.059	1.00	9.73
ATOM	1355	N	LEU	273	-10.272	9.247	19.238	1.00	10.93
ATOM	1356	CA	LEU	273	-11.260	10.111	19.864	1.00	9.70
ATOM	1357	CB	LEU	273	-11.112	11.565	19.403	1.00	8.30
ATOM	1358	CG	LEU	273	-11.635	12.024	18.038	1.00	9.20
ATOM	1359	CD1	LEU	273	-11.671	13.549	18.029	1.00	8.95
ATOM	1360	CD2	LEU	273	-10.760	11.506	16.908	1.00	5.31
ATOM	1361	C	LEU	273	-12.638	9.580	19.501	1.00	10.55
ATOM	1362	O	LEU	273	-12.795	8.865	18.512	1.00	8.35
ATOM	1363	N	LEU	274	-13.631	9.908	20.320	1.00	10.83
ATOM	1364	CA	LEU	274	-14.994	9.469	20.061	1.00	10.69
ATOM	1365	CB	LEU	274	-15.715	9.163	21.371	1.00	7.70
ATOM	1366	CG	LEU	274	-15.125	8.045	22.229	1.00	6.43
ATOM	1367	CD1	LEU	274	-15.966	7.902	23.494	1.00	6.40
ATOM	1368	CD2	LEU	274	-15.100	6.742	21.454	1.00	5.08
ATOM	1369	C	LEU	274	-15.757	10.558	19.329	1.00	9.94
ATOM	1370	O	LEU	274	-15.429	11.736	19.438	1.00	10.03
ATOM	1371	N	ALA	275	-16.775	10.155	18.581	1.00	12.87
ATOM	1372	CA	ALA	275	-17.595	11.108	17.857	1.00	11.71
ATOM	1373	CB	ALA	275	-18.726	10.388	17.135	1.00	11.59
ATOM	1374	C	ALA	275	-18.152	12.076	18.893	1.00	12.36
ATOM	1375	O	ALA	275	-18.398	13.237	18.590	1.00	11.70
ATOM	1376	N	GLU	276	-18.331	11.590	20.122	1.00	12.74
ATOM	1377	CA	GLU	276	-18.849	12.423	21.205	1.00	14.05
ATOM	1378	CB	GLU	276	-19.007	11.612	22.497	1.00	12.91
ATOM	1379	CG	GLU	276	-20.267	10.758	22.600	1.00	15.11
ATOM	1380	CD	GLU	276	-20.173	9.438	21.855	1.00	15.80
ATOM	1381	OE1	GLU	276	-20.992	8.536	22.153	1.00	16.05
ATOM	1382	OE2	GLU	276	-19.294	9.290	20.976	1.00	14.53
ATOM	1383	C	GLU	276	-17.943	13.623	21.480	1.00	14.00
ATOM	1384	O	GLU	276	-18.427	14.715	21.778	1.00	17.58
ATOM	1385	N	LEU	277	-16.630	13.422	21.396	1.00	14.75

ATOM	1386	CA	LEU	277	-15.690	14.514	21.633	1.00	13.38
ATOM	1387	CB	LEU	277	-14.262	13.995	21.829	1.00	11.48
ATOM	1388	CG	LEU	277	-13.221	15.117	21.961	1.00	10.61
ATOM	1389	CD1	LEU	277	-13.556	15.990	23.172	1.00	9.77
ATOM	1390	CD2	LEU	277	-11.820	14.525	22.098	1.00	10.28
ATOM	1391	C	LEU	277	-15.700	15.505	20.479	1.00	13.01
ATOM	1392	O	LEU	277	-15.669	16.720	20.693	1.00	12.41
ATOM	1393	N	TRP	278	-15.733	14.992	19.255	1.00	13.86
ATOM	1394	CA	TRP	278	-15.753	15.868	18.097	1.00	14.33
ATOM	1395	CB	TRP	278	-15.785	15.057	16.801	1.00	13.74
ATOM	1396	CG	TRP	278	-15.761	15.923	15.582	1.00	12.16
ATOM	1397	CD2	TRP	278	-14.771	16.903	15.253	1.00	11.89
ATOM	1398	CE2	TRP	278	-15.173	17.515	14.044	1.00	13.50
ATOM	1399	CE3	TRP	278	-13.582	17.327	15.865	1.00	12.06
ATOM	1400	CD1	TRP	278	-16.697	15.972	14.585	1.00	12.62
ATOM	1401	NE1	TRP	278	-16.351	16.929	13.657	1.00	12.72
ATOM	1402	CZ2	TRP	278	-14.428	18.530	13.434	1.00	13.08
ATOM	1403	CZ3	TRP	278	-12.842	18.337	15.260	1.00	9.94
ATOM	1404	CH2	TRP	278	-13.268	18.926	14.057	1.00	12.66
ATOM	1405	C	TRP	278	-16.971	16.788	18.164	1.00	15.62
ATOM	1406	O	TRP	278	-16.917	17.935	17.719	1.00	15.33
ATOM	1407	N	ALA	279	-18.071	16.281	18.718	1.00	16.90
ATOM	1408	CA	ALA	279	-19.291	17.074	18.853	1.00	15.07
ATOM	1409	CB	ALA	279	-20.428	16.202	19.386	1.00	16.52
ATOM	1410	C	ALA	279	-19.039	18.241	19.805	1.00	15.44
ATOM	1411	O	ALA	279	-19.622	19.318	19.666	1.00	13.86
ATOM	1412	N	GLU	280	-18.153	18.014	20.769	1.00	12.81
ATOM	1413	CA	GLU	280	-17.807	19.017	21.763	1.00	12.81
ATOM	1414	CB	GLU	280	-17.185	18.324	22.982	1.00	13.98
ATOM	1415	CG	GLU	280	-17.271	19.107	24.269	1.00	15.70
ATOM	1416	CD	GLU	280	-16.447	18.497	25.391	1.00	16.27
ATOM	1417	OE1	GLU	280	-16.525	17.270	25.606	1.00	13.55
ATOM	1418	OE2	GLU	280	-15.728	19.257	26.069	1.00	17.16
ATOM	1419	C	GLU	280	-16.820	20.057	21.219	1.00	12.01
ATOM	1420	O	GLU	280	-16.940	21.251	21.496	1.00	12.13
ATOM	1421	N	LEU	281	-15.855	19.594	20.430	1.00	12.30
ATOM	1422	CA	LEU	281	-14.808	20.460	19.895	1.00	11.56
ATOM	1423	CB	LEU	281	-13.536	19.634	19.676	1.00	11.64
ATOM	1424	CG	LEU	281	-13.022	18.859	20.899	1.00	9.87
ATOM	1425	CD1	LEU	281	-11.753	18.112	20.526	1.00	11.22
ATOM	1426	CD2	LEU	281	-12.761	19.815	22.057	1.00	11.75
ATOM	1427	C	LEU	281	-15.111	21.243	18.624	1.00	12.97
ATOM	1428	O	LEU	281	-14.845	22.445	18.552	1.00	11.59
ATOM	1429	N	GLU	282	-15.657	20.567	17.621	1.00	12.96
ATOM	1430	CA	GLU	282	-15.945	21.210	16.340	1.00	15.55
ATOM	1431	CB	GLU	282	-16.811	20.288	15.468	1.00	14.69
ATOM	1432	CG	GLU	282	-17.234	20.908	14.137	1.00	17.52
ATOM	1433	CD	GLU	282	-17.821	19.890	13.178	1.00	19.89
ATOM	1434	OE1	GLU	282	-17.111	19.481	12.232	1.00	23.75
ATOM	1435	OE2	GLU	282	-18.987	19.487	13.376	1.00	19.62
ATOM	1436	C	GLU	282	-16.579	22.603	16.404	1.00	15.53
ATOM	1437	O	GLU	282	-16.189	23.495	15.650	1.00	16.03
ATOM	1438	N	PRO	283	-17.557	22.811	17.299	1.00	15.91
ATOM	1439	CD	PRO	283	-18.213	21.835	18.188	1.00	16.18
ATOM	1440	CA	PRO	283	-18.204	24.123	17.403	1.00	14.91
ATOM	1441	CB	PRO	283	-19.256	23.908	18.492	1.00	16.00
ATOM	1442	CG	PRO	283	-19.575	22.450	18.380	1.00	15.67
ATOM	1443	C	PRO	283	-17.254	25.266	17.757	1.00	15.99
ATOM	1444	O	PRO	283	-17.489	26.416	17.384	1.00	16.84
ATOM	1445	N	LYS	284	-16.187	24.951	18.482	1.00	13.30
ATOM	1446	CA	LYS	284	-15.236	25.970	18.901	1.00	12.81
ATOM	1447	CB	LYS	284	-15.194	26.034	20.436	1.00	11.27

ATOM	1448	CG	LYS	284	-15.042	24.672	21.113	1.00	11.39
ATOM	1449	CD	LYS	284	-14.832	24.791	22.625	1.00	12.37
ATOM	1450	CE	LYS	284	-14.664	23.409	23.259	1.00	9.86
ATOM	1451	NZ	LYS	284	-14.221	23.487	24.676	1.00	9.76
ATOM	1452	C	LYS	284	-13.833	25.741	18.348	1.00	13.21
ATOM	1453	O	LYS	284	-12.865	26.302	18.866	1.00	13.63
ATOM	1454	N	TRP	285	-13.723	24.925	17.300	1.00	10.96
ATOM	1455	CA	TRP	285	-12.424	24.629	16.696	1.00	12.88
ATOM	1456	CB	TRP	285	-12.614	23.823	15.406	1.00	11.50
ATOM	1457	CG	TRP	285	-11.364	23.132	14.929	1.00	12.35
ATOM	1458	CD2	TRP	285	-10.716	22.011	15.545	1.00	10.54
ATOM	1459	CE2	TRP	285	-9.595	21.687	14.749	1.00	11.17
ATOM	1460	CE3	TRP	285	-10.975	21.248	16.694	1.00	13.32
ATOM	1461	CD1	TRP	285	-10.627	23.437	13.816	1.00	11.45
ATOM	1462	NE1	TRP	285	-9.564	22.571	13.702	1.00	11.53
ATOM	1463	CZ2	TRP	285	-8.731	20.631	15.064	1.00	10.57
ATOM	1464	CZ3	TRP	285	-10.112	20.193	17.010	1.00	11.31
ATOM	1465	CH2	TRP	285	-9.005	19.897	16.195	1.00	11.04
ATOM	1466	C	TRP	285	-11.654	25.928	16.407	1.00	13.07
ATOM	1467	O	TRP	285	-12.174	26.843	15.767	1.00	12.23
ATOM	1468	N	PRO	286	-10.392	26.010	16.866	1.00	14.09
ATOM	1469	CD	PRO	286	-9.650	24.903	17.502	1.00	14.48
ATOM	1470	CA	PRO	286	-9.522	27.179	16.691	1.00	13.63
ATOM	1471	CB	PRO	286	-8.393	26.901	17.670	1.00	13.42
ATOM	1472	CG	PRO	286	-8.212	25.420	17.504	1.00	14.99
ATOM	1473	C	PRO	286	-9.004	27.395	15.271	1.00	14.17
ATOM	1474	O	PRO	286	-9.080	26.500	14.431	1.00	13.38
ATOM	1475	N	LYS	287	-8.464	28.586	15.022	1.00	15.14
ATOM	1476	CA	LYS	287	-7.919	28.928	13.709	1.00	15.18
ATOM	1477	CB	LYS	287	-7.876	30.448	13.524	1.00	18.06
ATOM	1478	CG	LYS	287	-9.185	31.165	13.777	1.00	20.85
ATOM	1479	CD	LYS	287	-10.248	30.766	12.772	1.00	26.16
ATOM	1480	CE	LYS	287	-11.541	31.528	13.023	1.00	28.64
ATOM	1481	NZ	LYS	287	-12.569	31.232	11.988	1.00	31.39
ATOM	1482	C	LYS	287	-6.503	28.378	13.510	1.00	15.17
ATOM	1483	O	LYS	287	-6.037	28.267	12.369	1.00	12.52
ATOM	1484	N	ALA	288	-5.820	28.042	14.606	1.00	11.99
ATOM	1485	CA	ALA	288	-4.449	27.521	14.513	1.00	12.30
ATOM	1486	CB	ALA	288	-3.489	28.653	14.137	1.00	9.48
ATOM	1487	C	ALA	288	-3.965	26.856	15.798	1.00	12.77
ATOM	1488	O	ALA	288	-4.536	27.062	16.872	1.00	13.42
ATOM	1489	N	PHE	289	-2.890	26.078	15.676	1.00	12.29
ATOM	1490	CA	PHE	289	-2.291	25.378	16.810	1.00	12.01
ATOM	1491	CB	PHE	289	-1.604	26.394	17.721	1.00	13.36
ATOM	1492	CG	PHE	289	-0.818	27.436	16.969	1.00	15.85
ATOM	1493	CD1	PHE	289	-1.277	28.745	16.882	1.00	16.00
ATOM	1494	CD2	PHE	289	0.377	27.104	16.338	1.00	15.12
ATOM	1495	CE1	PHE	289	-0.561	29.713	16.179	1.00	16.99
ATOM	1496	CE2	PHE	289	1.101	28.063	15.634	1.00	16.27
ATOM	1497	CZ	PHE	289	0.630	29.372	15.555	1.00	17.28
ATOM	1498	C	PHE	289	-3.356	24.603	17.580	1.00	12.46
ATOM	1499	O	PHE	289	-3.544	24.795	18.790	1.00	11.25
ATOM	1500	N	TRP	290	-4.034	23.707	16.871	1.00	10.23
ATOM	1501	CA	TRP	290	-5.119	22.923	17.446	1.00	11.06
ATOM	1502	CB	TRP	290	-5.784	22.059	16.363	1.00	10.06
ATOM	1503	CG	TRP	290	-4.928	20.947	15.878	1.00	11.40
ATOM	1504	CD2	TRP	290	-4.814	19.646	16.464	1.00	11.49
ATOM	1505	CE2	TRP	290	-3.807	18.957	15.755	1.00	10.74
ATOM	1506	CE3	TRP	290	-5.458	19.000	17.528	1.00	10.68
ATOM	1507	CD1	TRP	290	-4.024	20.990	14.860	1.00	12.96
ATOM	1508	NE1	TRP	290	-3.343	19.797	14.779	1.00	12.26
ATOM	1509	CZ2	TRP	290	-3.426	17.647	16.075	1.00	9.83

ATOM	1510	CZ3	TRP	290	-5.080	17.700	17.847	1.00	11.32
ATOM	1511	CH2	TRP	290	-4.069	17.039	17.120	1.00	10.11
ATOM	1512	C	TRP	290	-4.748	22.046	18.639	1.00	11.85
ATOM	1513	O	TRP	290	-5.518	21.953	19.597	1.00	12.27
ATOM	1514	N	ASP	291	-3.579	21.411	18.592	1.00	12.07
ATOM	1515	CA	ASP	291	-3.159	20.538	19.684	1.00	11.73
ATOM	1516	CB	ASP	291	-1.938	19.712	19.272	1.00	14.91
ATOM	1517	CG	ASP	291	-0.823	20.555	18.703	1.00	16.60
ATOM	1518	OD1	ASP	291	0.303	20.041	18.638	1.00	17.64
ATOM	1519	OD2	ASP	291	-1.062	21.715	18.313	1.00	20.57
ATOM	1520	C	ASP	291	-2.889	21.247	21.010	1.00	11.51
ATOM	1521	O	ASP	291	-3.260	20.734	22.064	1.00	10.33
ATOM	1522	N	ASP	292	-2.239	22.407	20.978	1.00	9.27
ATOM	1523	CA	ASP	292	-1.984	23.132	22.220	1.00	12.31
ATOM	1524	CB	ASP	292	-0.943	24.235	22.015	1.00	10.62
ATOM	1525	CG	ASP	292	0.482	23.711	22.089	1.00	12.81
ATOM	1526	OD1	ASP	292	0.662	22.504	22.351	1.00	13.60
ATOM	1527	OD2	ASP	292	1.426	24.500	21.894	1.00	11.39
ATOM	1528	C	ASP	292	-3.290	23.727	22.725	1.00	11.93
ATOM	1529	O	ASP	292	-3.454	23.980	23.924	1.00	10.60
ATOM	1530	N	TRP	293	-4.220	23.934	21.796	1.00	11.80
ATOM	1531	CA	TRP	293	-5.547	24.467	22.114	1.00	11.49
ATOM	1532	CB	TRP	293	-6.293	24.785	20.821	1.00	12.11
ATOM	1533	CG	TRP	293	-7.734	25.135	20.991	1.00	12.28
ATOM	1534	CD2	TRP	293	-8.857	24.285	20.731	1.00	12.10
ATOM	1535	CE2	TRP	293	-10.023	25.045	20.977	1.00	13.02
ATOM	1536	CE3	TRP	293	-8.991	22.953	20.311	1.00	12.62
ATOM	1537	CD1	TRP	293	-8.248	26.338	21.383	1.00	14.87
ATOM	1538	NE1	TRP	293	-9.623	26.294	21.374	1.00	13.46
ATOM	1539	CZ2	TRP	293	-11.309	24.519	20.815	1.00	12.99
ATOM	1540	CZ3	TRP	293	-10.271	22.427	20.149	1.00	12.71
ATOM	1541	CH2	TRP	293	-11.414	23.213	20.401	1.00	15.12
ATOM	1542	C	TRP	293	-6.322	23.416	22.909	1.00	11.94
ATOM	1543	O	TRP	293	-7.039	23.734	23.861	1.00	11.88
ATOM	1544	N	MET	294	-6.183	22.157	22.512	1.00	10.79
ATOM	1545	CA	MET	294	-6.870	21.086	23.223	1.00	12.21
ATOM	1546	CB	MET	294	-6.817	19.783	22.421	1.00	13.06
ATOM	1547	CG	MET	294	-7.862	19.685	21.320	1.00	14.20
ATOM	1548	SD	MET	294	-7.713	18.155	20.402	1.00	20.72
ATOM	1549	CE	MET	294	-8.274	16.972	21.641	1.00	20.12
ATOM	1550	C	MET	294	-6.240	20.866	24.591	1.00	11.72
ATOM	1551	O	MET	294	-6.870	20.305	25.487	1.00	13.26
ATOM	1552	N	ARG	295	-4.997	21.312	24.751	1.00	9.90
ATOM	1553	CA	ARG	295	-4.296	21.150	26.014	1.00	11.49
ATOM	1554	CB	ARG	295	-2.783	21.252	25.791	1.00	11.19
ATOM	1555	CG	ARG	295	-2.182	19.954	25.263	1.00	13.56
ATOM	1556	CD	ARG	295	-0.909	20.169	24.452	1.00	14.54
ATOM	1557	NE	ARG	295	-0.452	18.911	23.863	1.00	14.95
ATOM	1558	CZ	ARG	295	0.417	18.825	22.862	1.00	15.59
ATOM	1559	NH1	ARG	295	0.932	19.926	22.327	1.00	16.67
ATOM	1560	NH2	ARG	295	0.772	17.638	22.393	1.00	18.28
ATOM	1561	C	ARG	295	-4.761	22.138	27.080	1.00	11.85
ATOM	1562	O	ARG	295	-4.440	21.987	28.259	1.00	13.01
ATOM	1563	N	ARG	296	-5.528	23.139	26.667	1.00	10.93
ATOM	1564	CA	ARG	296	-6.048	24.131	27.603	1.00	11.55
ATOM	1565	CB	ARG	296	-6.613	25.327	26.851	1.00	11.64
ATOM	1566	CG	ARG	296	-5.627	25.999	25.945	1.00	16.02
ATOM	1567	CD	ARG	296	-6.291	27.156	25.253	1.00	18.05
ATOM	1568	NE	ARG	296	-5.344	27.942	24.479	1.00	21.87
ATOM	1569	CZ	ARG	296	-5.689	29.000	23.753	1.00	24.13
ATOM	1570	NH1	ARG	296	-6.960	29.384	23.706	1.00	23.00
ATOM	1571	NH2	ARG	296	-4.768	29.678	23.088	1.00	23.52

ATOM	1572	C	ARG	296	-7.164	23.524	28.449	1.00	12.24
ATOM	1573	O	ARG	296	-7.901	22.649	27.990	1.00	10.72
ATOM	1574	N	PRO	297	-7.319	24.000	29.692	1.00	11.79
ATOM	1575	CD	PRO	297	-6.532	25.016	30.414	1.00	11.24
ATOM	1576	CA	PRO	297	-8.380	23.441	30.536	1.00	12.66
ATOM	1577	CB	PRO	297	-8.133	24.104	31.896	1.00	10.02
ATOM	1578	CG	PRO	297	-7.472	25.415	31.535	1.00	11.27
ATOM	1579	C	PRO	297	-9.794	23.675	29.992	1.00	13.99
ATOM	1580	O	PRO	297	-10.690	22.859	30.217	1.00	13.24
ATOM	1581	N	GLU	298	-9.994	24.775	29.267	1.00	13.51
ATOM	1582	CA	GLU	298	-11.310	25.075	28.707	1.00	13.82
ATOM	1583	CB	GLU	298	-11.285	26.381	27.902	1.00	16.58
ATOM	1584	CG	GLU	298	-10.994	27.641	28.705	1.00	20.51
ATOM	1585	CD	GLU	298	-9.598	27.647	29.299	1.00	22.90
ATOM	1586	OE1	GLU	298	-8.661	27.223	28.599	1.00	18.63
ATOM	1587	OE2	GLU	298	-9.439	28.086	30.460	1.00	27.03
ATOM	1588	C	GLU	298	-11.760	23.939	27.792	1.00	13.33
ATOM	1589	O	GLU	298	-12.952	23.702	27.623	1.00	10.93
ATOM	1590	N	GLN	299	-10.793	23.248	27.195	1.00	12.94
ATOM	1591	CA	GLN	299	-11.083	22.133	26.301	1.00	12.55
ATOM	1592	CB	GLN	299	-10.112	22.129	25.116	1.00	12.85
ATOM	1593	CG	GLN	299	-10.479	23.036	23.943	1.00	14.47
ATOM	1594	CD	GLN	299	-10.682	24.487	24.341	1.00	15.46
ATOM	1595	OE1	GLN	299	-11.796	24.905	24.660	1.00	16.09
ATOM	1596	NE2	GLN	299	-9.600	25.263	24.329	1.00	13.10
ATOM	1597	C	GLN	299	-10.964	20.796	27.024	1.00	12.12
ATOM	1598	O	GLN	299	-11.861	19.960	26.955	1.00	10.14
ATOM	1599	N	ARG	300	-9.841	20.606	27.710	1.00	12.21
ATOM	1600	CA	ARG	300	-9.561	19.363	28.422	1.00	13.28
ATOM	1601	CB	ARG	300	-8.156	19.425	29.030	1.00	12.57
ATOM	1602	CG	ARG	300	-7.631	18.085	29.518	1.00	14.18
ATOM	1603	CD	ARG	300	-6.140	18.166	29.832	1.00	15.25
ATOM	1604	NE	ARG	300	-5.860	18.790	31.122	1.00	17.96
ATOM	1605	CZ	ARG	300	-6.107	18.217	32.298	1.00	18.39
ATOM	1606	NH1	ARG	300	-6.644	17.002	32.350	1.00	16.43
ATOM	1607	NH2	ARG	300	-5.808	18.852	33.424	1.00	18.15
ATOM	1608	C	ARG	300	-10.574	19.049	29.512	1.00	12.10
ATOM	1609	O	ARG	300	-11.070	17.928	29.602	1.00	14.34
ATOM	1610	N	LYS	301	-10.859	20.040	30.349	1.00	13.70
ATOM	1611	CA	LYS	301	-11.807	19.876	31.441	1.00	11.84
ATOM	1612	CB	LYS	301	-13.214	19.668	30.876	1.00	11.97
ATOM	1613	CG	LYS	301	-13.762	20.877	30.124	1.00	13.06
ATOM	1614	CD	LYS	301	-15.037	20.534	29.368	1.00	12.37
ATOM	1615	CE	LYS	301	-15.579	21.730	28.601	1.00	17.56
ATOM	1616	NZ	LYS	301	-16.839	21.407	27.862	1.00	18.46
ATOM	1617	C	LYS	301	-11.429	18.713	32.365	1.00	12.77
ATOM	1618	O	LYS	301	-12.245	17.840	32.652	1.00	11.57
ATOM	1619	N	GLY	302	-10.176	18.702	32.806	1.00	12.60
ATOM	1620	CA	GLY	302	-9.708	17.673	33.720	1.00	14.37
ATOM	1621	C	GLY	302	-9.646	16.244	33.218	1.00	14.23
ATOM	1622	O	GLY	302	-9.251	15.348	33.962	1.00	14.57
ATOM	1623	N	ARG	303	-10.015	16.023	31.961	1.00	14.27
ATOM	1624	CA	ARG	303	-10.000	14.683	31.391	1.00	13.45
ATOM	1625	CB	ARG	303	-10.930	14.631	30.177	1.00	14.34
ATOM	1626	CG	ARG	303	-12.407	14.779	30.549	1.00	12.77
ATOM	1627	CD	ARG	303	-13.305	14.945	29.325	1.00	11.43
ATOM	1628	NE	ARG	303	-13.093	16.235	28.676	1.00	13.33
ATOM	1629	CZ	ARG	303	-13.876	16.736	27.722	1.00	13.78
ATOM	1630	NH1	ARG	303	-14.936	16.057	27.295	1.00	11.85
ATOM	1631	NH2	ARG	303	-13.606	17.925	27.203	1.00	13.00
ATOM	1632	C	ARG	303	-8.588	14.242	31.015	1.00	13.24
ATOM	1633	O	ARG	303	-7.707	15.071	30.774	1.00	12.59

ATOM	1634	N	ALA	304	-8.381	12.932	30.972	1.00	12.13
ATOM	1635	CA	ALA	304	-7.075	12.371	30.648	1.00	12.48
ATOM	1636	CB	ALA	304	-6.536	11.607	31.858	1.00	10.26
ATOM	1637	C	ALA	304	-7.101	11.447	29.437	1.00	10.78
ATOM	1638	O	ALA	304	-8.162	11.107	28.911	1.00	10.32
ATOM	1639	N	CYS	305	-5.914	11.056	28.986	1.00	11.56
ATOM	1640	CA	CYS	305	-5.791	10.128	27.870	1.00	11.86
ATOM	1641	C	CYS	305	-5.003	8.948	28.404	1.00	10.88
ATOM	1642	O	CYS	305	-4.340	9.039	29.436	1.00	10.30
ATOM	1643	CB	CYS	305	-4.957	10.682	26.706	1.00	13.24
ATOM	1644	SG	CYS	305	-5.497	12.087	25.680	1.00	16.80
ATOM	1645	N	VAL	306	-5.066	7.842	27.684	1.00	9.86
ATOM	1646	CA	VAL	306	-4.288	6.678	28.051	1.00	10.31
ATOM	1647	CB	VAL	306	-5.026	5.360	27.711	1.00	7.61
ATOM	1648	CG1	VAL	306	-4.063	4.181	27.818	1.00	8.43
ATOM	1649	CG2	VAL	306	-6.201	5.162	28.666	1.00	10.37
ATOM	1650	C	VAL	306	-3.070	6.808	27.156	1.00	9.36
ATOM	1651	O	VAL	306	-3.191	7.248	26.013	1.00	11.01
ATOM	1652	N	ARG	307	-1.897	6.483	27.686	1.00	9.40
ATOM	1653	CA	ARG	307	-0.664	6.518	26.905	1.00	7.88
ATOM	1654	CB	ARG	307	0.094	7.846	27.107	1.00	9.00
ATOM	1655	CG	ARG	307	0.667	8.105	28.492	1.00	10.22
ATOM	1656	CD	ARG	307	2.034	7.465	28.638	1.00	9.89
ATOM	1657	NE	ARG	307	2.626	7.739	29.947	1.00	11.94
ATOM	1658	CZ	ARG	307	3.798	7.255	30.343	1.00	12.16
ATOM	1659	NH1	ARG	307	4.500	6.475	29.528	1.00	8.07
ATOM	1660	NH2	ARG	307	4.258	7.539	31.552	1.00	9.31
ATOM	1661	C	ARG	307	0.139	5.304	27.382	1.00	8.79
ATOM	1662	O	ARG	307	-0.021	4.857	28.516	1.00	7.16
ATOM	1663	N	PRO	308	0.997	4.746	26.516	1.00	9.49
ATOM	1664	CD	PRO	308	1.141	5.053	25.079	1.00	9.36
ATOM	1665	CA	PRO	308	1.796	3.572	26.875	1.00	8.14
ATOM	1666	CB	PRO	308	1.844	2.808	25.569	1.00	8.93
ATOM	1667	CG	PRO	308	2.080	3.935	24.587	1.00	10.06
ATOM	1668	C	PRO	308	3.199	3.863	27.382	1.00	8.79
ATOM	1669	O	PRO	308	3.718	4.961	27.201	1.00	5.24
ATOM	1670	N	GLU	309	3.810	2.852	27.996	1.00	7.59
ATOM	1671	CA	GLU	309	5.178	2.953	28.493	1.00	8.40
ATOM	1672	CB	GLU	309	5.542	1.682	29.270	1.00	10.62
ATOM	1673	CG	GLU	309	7.027	1.514	29.630	1.00	9.63
ATOM	1674	CD	GLU	309	7.456	2.338	30.826	1.00	12.95
ATOM	1675	OE1	GLU	309	6.601	3.030	31.418	1.00	14.08
ATOM	1676	OE2	GLU	309	8.657	2.289	31.178	1.00	11.21
ATOM	1677	C	GLU	309	6.095	3.097	27.275	1.00	9.22
ATOM	1678	O	GLU	309	7.059	3.868	27.296	1.00	8.50
ATOM	1679	N	ILE	310	5.783	2.339	26.221	1.00	9.16
ATOM	1680	CA	ILE	310	6.547	2.347	24.971	1.00	8.07
ATOM	1681	CB	ILE	310	7.112	0.935	24.660	1.00	6.00
ATOM	1682	CG2	ILE	310	7.910	0.955	23.358	1.00	8.37
ATOM	1683	CG1	ILE	310	8.000	0.468	25.814	1.00	8.79
ATOM	1684	CD1	ILE	310	8.638	-0.914	25.600	1.00	10.24
ATOM	1685	C	ILE	310	5.598	2.788	23.850	1.00	8.59
ATOM	1686	O	ILE	310	4.539	2.189	23.654	1.00	9.12
ATOM	1687	N	SER	311	5.983	3.833	23.121	1.00	10.06
ATOM	1688	CA	SER	311	5.146	4.391	22.055	1.00	10.45
ATOM	1689	CB	SER	311	5.834	5.609	21.428	1.00	10.65
ATOM	1690	OG	SER	311	6.136	6.592	22.403	1.00	15.67
ATOM	1691	C	SER	311	4.753	3.414	20.948	1.00	11.04
ATOM	1692	O	SER	311	5.527	2.530	20.572	1.00	10.30
ATOM	1693	N	ARG	312	3.537	3.578	20.432	1.00	9.47
ATOM	1694	CA	ARG	312	3.053	2.726	19.353	1.00	9.38
ATOM	1695	CB	ARG	312	1.614	2.276	19.622	1.00	8.94

ATOM	1696	CG	ARG	312	1.542	0.826	20.129	1.00	9.00
ATOM	1697	CD	ARG	312	2.366	0.656	21.407	1.00	9.14
ATOM	1698	NE	ARG	312	2.451	-0.740	21.836	1.00	9.60
ATOM	1699	CZ	ARG	312	2.868	-1.127	23.039	1.00	8.93
ATOM	1700	NH1	ARG	312	3.237	-0.223	23.932	1.00	12.61
ATOM	1701	NH2	ARG	312	2.909	-2.414	23.356	1.00	7.21
ATOM	1702	C	ARG	312	3.167	3.429	18.007	1.00	8.31
ATOM	1703	O	ARG	312	2.696	2.933	16.984	1.00	10.05
ATOM	1704	N	THR	313	3.791	4.603	18.027	1.00	7.29
ATOM	1705	CA	THR	313	4.049	5.376	16.814	1.00	8.77
ATOM	1706	CB	THR	313	3.010	6.487	16.552	1.00	8.81
ATOM	1707	OG1	THR	313	2.900	7.317	17.711	1.00	7.00
ATOM	1708	CG2	THR	313	1.663	5.893	16.188	1.00	5.83
ATOM	1709	C	THR	313	5.388	6.061	17.013	1.00	9.15
ATOM	1710	O	THR	313	5.870	6.188	18.139	1.00	6.76
ATOM	1711	N	MET	314	5.980	6.498	15.910	1.00	10.65
ATOM	1712	CA	MET	314	7.253	7.198	15.923	1.00	12.80
ATOM	1713	CB	MET	314	8.414	6.220	15.716	1.00	15.65
ATOM	1714	CG	MET	314	8.329	5.453	14.400	1.00	21.19
ATOM	1715	SD	MET	314	9.953	5.072	13.742	1.00	30.08
ATOM	1716	CE	MET	314	10.466	6.686	13.200	1.00	25.92
ATOM	1717	C	MET	314	7.162	8.140	14.736	1.00	13.23
ATOM	1718	O	MET	314	6.430	7.864	13.783	1.00	13.00
ATOM	1719	N	THR	315	7.885	9.251	14.780	1.00	11.88
ATOM	1720	CA	THR	315	7.830	10.181	13.667	1.00	13.36
ATOM	1721	CB	THR	315	7.388	11.607	14.118	1.00	13.00
ATOM	1722	OG1	THR	315	7.257	12.454	12.968	1.00	14.28
ATOM	1723	CG2	THR	315	8.400	12.222	15.076	1.00	10.77
ATOM	1724	C	THR	315	9.158	10.273	12.925	1.00	14.65
ATOM	1725	O	THR	315	10.233	10.223	13.526	1.00	14.47
ATOM	1726	N	PHE	316	9.065	10.383	11.606	1.00	16.15
ATOM	1727	CA	PHE	316	10.240	10.510	10.756	1.00	16.54
ATOM	1728	CB	PHE	316	10.344	9.318	9.800	1.00	16.04
ATOM	1729	CG	PHE	316	9.079	9.036	9.030	1.00	15.20
ATOM	1730	CD1	PHE	316	8.158	8.107	9.499	1.00	14.07
ATOM	1731	CD2	PHE	316	8.811	9.706	7.839	1.00	14.77
ATOM	1732	CE1	PHE	316	6.996	7.847	8.795	1.00	15.06
ATOM	1733	CE2	PHE	316	7.640	9.454	7.126	1.00	12.72
ATOM	1734	CZ	PHE	316	6.727	8.521	7.607	1.00	14.63
ATOM	1735	C	PHE	316	10.135	11.817	9.967	1.00	17.90
ATOM	1736	O	PHE	316	10.970	12.112	9.117	1.00	18.29
ATOM	1737	N	GLY	317	9.107	12.604	10.275	1.00	19.81
ATOM	1738	CA	GLY	317	8.894	13.872	9.593	1.00	20.94
ATOM	1739	C	GLY	317	9.853	14.993	9.959	1.00	23.48
ATOM	1740	O	GLY	317	9.463	15.981	10.600	1.00	21.55
ATOM	1741	N	ARG	318	11.108	14.843	9.542	1.00	25.03
ATOM	1742	CA	ARG	318	12.152	15.831	9.795	1.00	26.80
ATOM	1743	CB	ARG	318	13.450	15.400	9.109	1.00	30.61
ATOM	1744	CG	ARG	318	14.009	14.085	9.616	1.00	35.71
ATOM	1745	CD	ARG	318	15.320	13.735	8.928	1.00	38.71
ATOM	1746	NE	ARG	318	16.017	12.647	9.611	1.00	41.21
ATOM	1747	CZ	ARG	318	16.501	12.732	10.847	1.00	42.86
ATOM	1748	NH1	ARG	318	16.365	13.856	11.540	1.00	44.80
ATOM	1749	NH2	ARG	318	17.124	11.696	11.390	1.00	43.48
ATOM	1750	C	ARG	318	11.736	17.197	9.260	1.00	26.34
ATOM	1751	O	ARG	318	11.775	18.203	9.973	1.00	24.27
ATOM	1752	N	LYS	319	11.341	17.211	7.992	1.00	25.56
ATOM	1753	CA	LYS	319	10.908	18.424	7.309	1.00	24.68
ATOM	1754	CB	LYS	319	11.462	18.430	5.877	1.00	26.04
ATOM	1755	CG	LYS	319	10.883	19.494	4.953	1.00	25.16
ATOM	1756	CD	LYS	319	11.285	20.900	5.365	1.00	26.68
ATOM	1757	CE	LYS	319	10.682	21.923	4.418	1.00	25.37

ATOM	1758	NZ	LYS	319	9.193	21.815	4.398	1.00	22.99
ATOM	1759	C	LYS	319	9.383	18.460	7.287	1.00	23.97
ATOM	1760	O	LYS	319	8.739	17.492	6.881	1.00	23.96
ATOM	1761	N	GLY	320	8.813	19.574	7.734	1.00	23.36
ATOM	1762	CA	GLY	320	7.368	19.713	7.752	1.00	22.45
ATOM	1763	C	GLY	320	6.948	21.156	7.945	1.00	23.10
ATOM	1764	O	GLY	320	7.625	22.077	7.474	1.00	21.49
ATOM	1765	N	VAL	321	5.826	21.364	8.625	1.00	22.45
ATOM	1766	CA	VAL	321	5.349	22.717	8.881	1.00	25.54
ATOM	1767	CB	VAL	321	3.923	22.709	9.461	1.00	24.90
ATOM	1768	CG1	VAL	321	3.514	24.114	9.880	1.00	24.57
ATOM	1769	CG2	VAL	321	2.960	22.171	8.425	1.00	25.23
ATOM	1770	C	VAL	321	6.294	23.373	9.878	1.00	28.20
ATOM	1771	O	VAL	321	6.991	24.336	9.547	1.00	28.59
ATOM	1772	N	SER	322	6.318	22.843	11.096	1.00	30.83
ATOM	1773	CA	SER	322	7.191	23.369	12.139	1.00	34.55
ATOM	1774	CB	SER	322	6.938	22.657	13.473	1.00	34.83
ATOM	1775	OG	SER	322	5.572	22.705	13.847	1.00	36.93
ATOM	1776	C	SER	322	8.643	23.145	11.740	1.00	36.06
ATOM	1777	O	SER	322	8.941	22.341	10.852	1.00	36.33
ATOM	1778	N	HIS	323	9.543	23.863	12.401	1.00	37.55
ATOM	1779	CA	HIS	323	10.966	23.722	12.134	1.00	38.63
ATOM	1780	CB	HIS	323	11.732	24.895	12.749	1.00	42.03
ATOM	1781	CG	HIS	323	11.222	26.234	12.314	1.00	45.05
ATOM	1782	CD2	HIS	323	10.813	27.310	13.028	1.00	46.58
ATOM	1783	ND1	HIS	323	11.069	26.576	10.986	1.00	46.36
ATOM	1784	CE1	HIS	323	10.588	27.803	10.902	1.00	47.43
ATOM	1785	NE2	HIS	323	10.423	28.272	12.127	1.00	47.83
ATOM	1786	C	HIS	323	11.411	22.397	12.749	1.00	37.13
ATOM	1787	O	HIS	323	10.723	21.843	13.609	1.00	36.17
ATOM	1788	N	GLY	324	12.557	21.888	12.307	1.00	35.66
ATOM	1789	CA	GLY	324	13.033	20.615	12.815	1.00	34.34
ATOM	1790	C	GLY	324	13.812	20.611	14.119	1.00	32.79
ATOM	1791	O	GLY	324	14.488	19.625	14.414	1.00	33.25
ATOM	1792	N	GLN	325	13.728	21.678	14.909	1.00	30.72
ATOM	1793	CA	GLN	325	14.473	21.709	16.165	1.00	28.26
ATOM	1794	CB	GLN	325	14.602	23.138	16.698	1.00	29.35
ATOM	1795	CG	GLN	325	15.451	23.227	17.963	1.00	31.96
ATOM	1796	CD	GLN	325	16.001	24.622	18.213	1.00	35.22
ATOM	1797	OE1	GLN	325	15.247	25.584	18.369	1.00	36.55
ATOM	1798	NE2	GLN	325	17.326	24.735	18.248	1.00	34.26
ATOM	1799	C	GLN	325	13.861	20.816	17.233	1.00	26.23
ATOM	1800	O	GLN	325	14.568	20.038	17.876	1.00	25.89
ATOM	1801	N	PHE	326	12.553	20.924	17.431	1.00	24.15
ATOM	1802	CA	PHE	326	11.892	20.095	18.423	1.00	21.87
ATOM	1803	CB	PHE	326	10.418	20.486	18.568	1.00	22.77
ATOM	1804	CG	PHE	326	9.714	19.769	19.685	1.00	23.85
ATOM	1805	CD1	PHE	326	10.219	19.813	20.982	1.00	23.82
ATOM	1806	CD2	PHE	326	8.563	19.029	19.441	1.00	23.19
ATOM	1807	CE1	PHE	326	9.590	19.129	22.017	1.00	23.39
ATOM	1808	CE2	PHE	326	7.927	18.340	20.473	1.00	23.50
ATOM	1809	CZ	PHE	326	8.442	18.390	21.761	1.00	23.94
ATOM	1810	C	PHE	326	12.009	18.637	17.990	1.00	21.11
ATOM	1811	O	PHE	326	12.173	17.746	18.825	1.00	19.99
ATOM	1812	N	PHE	327	11.938	18.402	16.682	1.00	18.59
ATOM	1813	CA	PHE	327	12.051	17.050	16.136	1.00	19.66
ATOM	1814	CB	PHE	327	11.693	17.026	14.642	1.00	19.26
ATOM	1815	CG	PHE	327	11.943	15.689	13.982	1.00	20.87
ATOM	1816	CD1	PHE	327	10.923	14.746	13.876	1.00	21.37
ATOM	1817	CD2	PHE	327	13.218	15.352	13.524	1.00	20.18
ATOM	1818	CE1	PHE	327	11.166	13.483	13.329	1.00	21.89
ATOM	1819	CE2	PHE	327	13.477	14.095	12.976	1.00	21.16

ATOM	1820	CZ	PHE	327	12.448	13.155	12.878	1.00	21.60
ATOM	1821	C	PHE	327	13.474	16.521	16.296	1.00	20.03
ATOM	1822	O	PHE	327	13.678	15.347	16.621	1.00	18.89
ATOM	1823	N	ASP	328	14.452	17.391	16.053	1.00	19.38
ATOM	1824	CA	ASP	328	15.856	17.009	16.137	1.00	20.88
ATOM	1825	CB	ASP	328	16.746	18.057	15.451	1.00	22.19
ATOM	1826	CG	ASP	328	16.802	17.881	13.941	1.00	25.23
ATOM	1827	OD1	ASP	328	16.772	16.721	13.474	1.00	24.02
ATOM	1828	OD2	ASP	328	16.898	18.901	13.222	1.00	26.95
ATOM	1829	C	ASP	328	16.376	16.777	17.545	1.00	20.28
ATOM	1830	O	ASP	328	17.257	15.943	17.754	1.00	19.05
ATOM	1831	N	GLN	329	15.838	17.505	18.514	1.00	19.63
ATOM	1832	CA	GLN	329	16.306	17.356	19.884	1.00	20.90
ATOM	1833	CB	GLN	329	16.453	18.728	20.538	1.00	21.89
ATOM	1834	CG	GLN	329	17.513	19.600	19.889	1.00	25.25
ATOM	1835	CD	GLN	329	17.745	20.883	20.653	1.00	26.64
ATOM	1836	OE1	GLN	329	16.832	21.693	20.819	1.00	28.83
ATOM	1837	NE2	GLN	329	18.971	21.076	21.127	1.00	27.73
ATOM	1838	C	GLN	329	15.430	16.472	20.753	1.00	19.85
ATOM	1839	O	GLN	329	15.856	16.035	21.821	1.00	18.82
ATOM	1840	N	HIS	330	14.216	16.188	20.301	1.00	16.80
ATOM	1841	CA	HIS	330	13.337	15.361	21.109	1.00	17.44
ATOM	1842	CB	HIS	330	12.360	16.244	21.880	1.00	17.84
ATOM	1843	CG	HIS	330	11.420	15.473	22.750	1.00	18.79
ATOM	1844	CD2	HIS	330	10.099	15.205	22.619	1.00	18.31
ATOM	1845	ND1	HIS	330	11.830	14.831	23.901	1.00	20.50
ATOM	1846	CE1	HIS	330	10.802	14.201	24.440	1.00	19.83
ATOM	1847	NE2	HIS	330	9.739	14.411	23.681	1.00	19.45
ATOM	1848	C	HIS	330	12.539	14.276	20.394	1.00	15.89
ATOM	1849	O	HIS	330	12.723	13.085	20.656	1.00	15.10
ATOM	1850	N	LEU	331	11.646	14.696	19.504	1.00	15.12
ATOM	1851	CA	LEU	331	10.775	13.777	18.787	1.00	12.29
ATOM	1852	CB	LEU	331	9.926	14.547	17.776	1.00	12.94
ATOM	1853	CG	LEU	331	8.966	15.600	18.339	1.00	14.35
ATOM	1854	CD1	LEU	331	8.284	16.300	17.182	1.00	17.03
ATOM	1855	CD2	LEU	331	7.936	14.955	19.256	1.00	12.67
ATOM	1856	C	LEU	331	11.436	12.597	18.090	1.00	11.92
ATOM	1857	O	LEU	331	10.893	11.492	18.111	1.00	10.11
ATOM	1858	N	LYS	332	12.596	12.821	17.476	1.00	11.07
ATOM	1859	CA	LYS	332	13.279	11.751	16.754	1.00	10.90
ATOM	1860	CB	LYS	332	14.458	12.312	15.938	1.00	13.83
ATOM	1861	CG	LYS	332	15.640	12.810	16.786	1.00	16.82
ATOM	1862	CD	LYS	332	16.830	13.261	15.926	1.00	17.91
ATOM	1863	CE	LYS	332	17.569	12.075	15.323	1.00	20.07
ATOM	1864	NZ	LYS	332	18.804	12.488	14.583	1.00	20.10
ATOM	1865	C	LYS	332	13.791	10.637	17.660	1.00	10.47
ATOM	1866	O	LYS	332	14.102	9.549	17.186	1.00	10.93
ATOM	1867	N	PHE	333	13.874	10.895	18.959	1.00	11.12
ATOM	1868	CA	PHE	333	14.391	9.882	19.877	1.00	11.48
ATOM	1869	CB	PHE	333	15.254	10.549	20.951	1.00	13.10
ATOM	1870	CG	PHE	333	16.436	11.281	20.387	1.00	13.67
ATOM	1871	CD1	PHE	333	16.512	12.668	20.454	1.00	12.34
ATOM	1872	CD2	PHE	333	17.447	10.583	19.729	1.00	14.41
ATOM	1873	CE1	PHE	333	17.575	13.355	19.868	1.00	12.53
ATOM	1874	CE2	PHE	333	18.514	11.257	19.140	1.00	14.58
ATOM	1875	CZ	PHE	333	18.576	12.648	19.209	1.00	12.27
ATOM	1876	C	PHE	333	13.343	8.989	20.530	1.00	11.51
ATOM	1877	O	PHE	333	13.691	8.060	21.259	1.00	7.89
ATOM	1878	N	ILE	334	12.069	9.259	20.260	1.00	10.59
ATOM	1879	CA	ILE	334	10.995	8.454	20.828	1.00	14.68
ATOM	1880	CB	ILE	334	9.630	9.159	20.653	1.00	14.72
ATOM	1881	CG2	ILE	334	8.517	8.326	21.255	1.00	15.09

ATOM	1882	CG1	ILE	334	9.679	10.533	21.326	1.00	18.02
ATOM	1883	CD1	ILE	334	10.025	10.496	22.807	1.00	19.85
ATOM	1884	C	ILE	334	10.994	7.091	20.140	1.00	14.78
ATOM	1885	O	ILE	334	10.777	6.989	18.931	1.00	16.14
ATOM	1886	N	LYS	335	11.247	6.051	20.928	1.00	16.41
ATOM	1887	CA	LYS	335	11.326	4.673	20.447	1.00	17.50
ATOM	1888	CB	LYS	335	12.033	3.823	21.510	1.00	21.51
ATOM	1889	CG	LYS	335	12.071	2.326	21.234	1.00	26.07
ATOM	1890	CD	LYS	335	12.709	1.587	22.406	1.00	29.71
ATOM	1891	CE	LYS	335	12.623	0.076	22.242	1.00	32.06
ATOM	1892	NZ	LYS	335	13.329	-0.404	21.023	1.00	32.54
ATOM	1893	C	LYS	335	9.999	4.012	20.069	1.00	16.08
ATOM	1894	O	LYS	335	9.001	4.125	20.783	1.00	14.22
ATOM	1895	N	LEU	336	9.999	3.307	18.942	1.00	15.53
ATOM	1896	CA	LEU	336	8.802	2.605	18.485	1.00	13.84
ATOM	1897	CB	LEU	336	8.781	2.516	16.956	1.00	15.33
ATOM	1898	CG	LEU	336	7.555	1.837	16.328	1.00	15.30
ATOM	1899	CD1	LEU	336	6.310	2.650	16.650	1.00	12.28
ATOM	1900	CD2	LEU	336	7.732	1.728	14.813	1.00	11.38
ATOM	1901	C	LEU	336	8.782	1.198	19.063	1.00	14.42
ATOM	1902	O	LEU	336	9.775	0.469	18.972	1.00	15.70
ATOM	1903	N	ASN	337	7.657	0.810	19.656	1.00	13.30
ATOM	1904	CA	ASN	337	7.535	-0.527	20.217	1.00	13.41
ATOM	1905	CB	ASN	337	6.182	-0.699	20.912	1.00	12.12
ATOM	1906	CG	ASN	337	6.020	-2.074	21.519	1.00	11.55
ATOM	1907	OD1	ASN	337	6.794	-2.473	22.389	1.00	13.55
ATOM	1908	ND2	ASN	337	5.017	-2.810	21.060	1.00	8.19
ATOM	1909	C	ASN	337	7.676	-1.578	19.119	1.00	15.01
ATOM	1910	O	ASN	337	7.140	-1.417	18.018	1.00	13.86
ATOM	1911	N	GLN	338	8.396	-2.653	19.427	1.00	15.85
ATOM	1912	CA	GLN	338	8.619	-3.730	18.470	1.00	18.25
ATOM	1913	CB	GLN	338	10.116	-3.882	18.188	1.00	21.65
ATOM	1914	CG	GLN	338	10.746	-2.660	17.533	1.00	27.69
ATOM	1915	CD	GLN	338	10.158	-2.358	16.165	1.00	30.34
ATOM	1916	OE1	GLN	338	10.491	-1.349	15.543	1.00	34.83
ATOM	1917	NE2	GLN	338	9.281	-3.236	15.689	1.00	31.44
ATOM	1918	C	GLN	338	8.058	-5.069	18.939	1.00	17.53
ATOM	1919	O	GLN	338	7.865	-5.975	18.135	1.00	17.97
ATOM	1920	N	GLN	339	7.806	-5.201	20.237	1.00	15.76
ATOM	1921	CA	GLN	339	7.268	-6.451	20.764	1.00	14.91
ATOM	1922	CB	GLN	339	7.836	-6.751	22.157	1.00	17.40
ATOM	1923	CG	GLN	339	7.315	-8.061	22.742	1.00	23.41
ATOM	1924	CD	GLN	339	7.984	-8.449	24.050	1.00	26.89
ATOM	1925	OE1	GLN	339	7.642	-9.472	24.652	1.00	29.87
ATOM	1926	NE2	GLN	339	8.942	-7.641	24.496	1.00	26.27
ATOM	1927	C	GLN	339	5.750	-6.373	20.829	1.00	12.70
ATOM	1928	O	GLN	339	5.189	-5.524	21.527	1.00	10.10
ATOM	1929	N	PHE	340	5.094	-7.261	20.089	1.00	11.33
ATOM	1930	CA	PHE	340	3.640	-7.296	20.035	1.00	11.93
ATOM	1931	CB	PHE	340	3.164	-8.272	18.950	1.00	9.13
ATOM	1932	CG	PHE	340	1.677	-8.244	18.726	1.00	9.16
ATOM	1933	CD1	PHE	340	1.127	-7.456	17.717	1.00	10.09
ATOM	1934	CD2	PHE	340	0.823	-8.960	19.556	1.00	11.24
ATOM	1935	CE1	PHE	340	-0.250	-7.377	17.542	1.00	6.38
ATOM	1936	CE2	PHE	340	-0.558	-8.888	19.391	1.00	11.09
ATOM	1937	CZ	PHE	340	-1.095	-8.095	18.382	1.00	12.06
ATOM	1938	C	PHE	340	3.027	-7.707	21.366	1.00	10.98
ATOM	1939	O	PHE	340	3.334	-8.771	21.899	1.00	10.18
ATOM	1940	N	VAL	341	2.153	-6.856	21.891	1.00	9.99
ATOM	1941	CA	VAL	341	1.465	-7.131	23.144	1.00	8.08
ATOM	1942	CB	VAL	341	1.563	-5.929	24.113	1.00	8.45
ATOM	1943	CG1	VAL	341	0.740	-6.202	25.367	1.00	9.42

ATOM	1944	CG2	VAL	341	3.020	-5.667	24.481	1.00	6.53
ATOM	1945	C	VAL	341	-0.012	-7.383	22.817	1.00	9.63
ATOM	1946	O	VAL	341	-0.657	-6.559	22.162	1.00	8.38
ATOM	1947	N	PRO	342	-0.559	-8.534	23.243	1.00	8.89
ATOM	1948	CD	PRO	342	0.084	-9.668	23.936	1.00	8.68
ATOM	1949	CA	PRO	342	-1.969	-8.825	22.962	1.00	9.24
ATOM	1950	CB	PRO	342	-2.053	-10.337	23.159	1.00	7.94
ATOM	1951	CG	PRO	342	-1.115	-10.560	24.302	1.00	6.57
ATOM	1952	C	PRO	342	-2.877	-8.065	23.934	1.00	7.98
ATOM	1953	O	PRO	342	-3.531	-8.671	24.784	1.00	10.70
ATOM	1954	N	PHE	343	-2.910	-6.741	23.804	1.00	8.97
ATOM	1955	CA	PHE	343	-3.732	-5.908	24.679	1.00	7.44
ATOM	1956	CB	PHE	343	-3.730	-4.445	24.220	1.00	7.91
ATOM	1957	CG	PHE	343	-2.430	-3.722	24.464	1.00	8.27
ATOM	1958	CD1	PHE	343	-1.543	-3.489	23.420	1.00	8.46
ATOM	1959	CD2	PHE	343	-2.116	-3.239	25.729	1.00	8.30
ATOM	1960	CE1	PHE	343	-0.363	-2.779	23.631	1.00	10.11
ATOM	1961	CE2	PHE	343	-0.939	-2.530	25.952	1.00	10.97
ATOM	1962	CZ	PHE	343	-0.061	-2.297	24.902	1.00	8.08
ATOM	1963	C	PHE	343	-5.173	-6.373	24.797	1.00	8.71
ATOM	1964	O	PHE	343	-5.769	-6.238	25.866	1.00	7.12
ATOM	1965	N	THR	344	-5.743	-6.909	23.718	1.00	7.51
ATOM	1966	CA	THR	344	-7.131	-7.376	23.779	1.00	9.69
ATOM	1967	CB	THR	344	-7.697	-7.748	22.374	1.00	9.08
ATOM	1968	OG1	THR	344	-6.945	-8.829	21.809	1.00	13.42
ATOM	1969	CG2	THR	344	-7.643	-6.543	21.438	1.00	10.33
ATOM	1970	C	THR	344	-7.314	-8.573	24.720	1.00	11.50
ATOM	1971	O	THR	344	-8.440	-8.898	25.101	1.00	11.32
ATOM	1972	N	GLN	345	-6.215	-9.215	25.113	1.00	11.97
ATOM	1973	CA	GLN	345	-6.290	-10.365	26.021	1.00	10.36
ATOM	1974	CB	GLN	345	-5.310	-11.463	25.594	1.00	11.78
ATOM	1975	CG	GLN	345	-5.523	-12.052	24.195	1.00	11.91
ATOM	1976	CD	GLN	345	-4.483	-13.116	23.878	1.00	14.76
ATOM	1977	OE1	GLN	345	-3.432	-13.163	24.514	1.00	13.98
ATOM	1978	NE2	GLN	345	-4.764	-13.964	22.889	1.00	13.27
ATOM	1979	C	GLN	345	-5.954	-9.960	27.457	1.00	12.23
ATOM	1980	O	GLN	345	-5.921	-10.795	28.359	1.00	11.22
ATOM	1981	N	LEU	346	-5.719	-8.673	27.666	1.00	11.87
ATOM	1982	CA	LEU	346	-5.349	-8.161	28.980	1.00	12.41
ATOM	1983	CB	LEU	346	-4.174	-7.205	28.808	1.00	12.68
ATOM	1984	CG	LEU	346	-3.042	-7.819	27.986	1.00	13.31
ATOM	1985	CD1	LEU	346	-1.928	-6.812	27.778	1.00	12.89
ATOM	1986	CD2	LEU	346	-2.525	-9.044	28.702	1.00	11.46
ATOM	1987	C	LEU	346	-6.469	-7.457	29.746	1.00	12.48
ATOM	1988	O	LEU	346	-7.440	-6.994	29.156	1.00	13.97
ATOM	1989	N	ASP	347	-6.310	-7.364	31.065	1.00	11.50
ATOM	1990	CA	ASP	347	-7.294	-6.714	31.929	1.00	11.90
ATOM	1991	CB	ASP	347	-7.346	-7.390	33.304	1.00	12.47
ATOM	1992	CG	ASP	347	-8.432	-6.819	34.194	1.00	17.32
ATOM	1993	OD1	ASP	347	-8.858	-5.668	33.949	1.00	15.32
ATOM	1994	OD2	ASP	347	-8.853	-7.522	35.145	1.00	17.61
ATOM	1995	C	ASP	347	-6.863	-5.271	32.118	1.00	12.21
ATOM	1996	O	ASP	347	-6.032	-4.983	32.979	1.00	10.38
ATOM	1997	N	LEU	348	-7.421	-4.366	31.322	1.00	11.56
ATOM	1998	CA	LEU	348	-7.064	-2.957	31.416	1.00	13.74
ATOM	1999	CB	LEU	348	-7.173	-2.293	30.035	1.00	14.79
ATOM	2000	CG	LEU	348	-6.576	-3.023	28.826	1.00	13.77
ATOM	2001	CD1	LEU	348	-6.741	-2.172	27.571	1.00	14.06
ATOM	2002	CD2	LEU	348	-5.119	-3.303	29.060	1.00	13.73
ATOM	2003	C	LEU	348	-7.948	-2.187	32.400	1.00	15.03
ATOM	2004	O	LEU	348	-8.051	-0.967	32.305	1.00	12.96
ATOM	2005	N	SER	349	-8.578	-2.881	33.344	1.00	16.06

ATOM	2006	CA	SER	349	-9.456	-2.193	34.291	1.00	16.27
ATOM	2007	CB	SER	349	-10.304	-3.201	35.080	1.00	16.57
ATOM	2008	OG	SER	349	-9.506	-4.003	35.928	1.00	17.19
ATOM	2009	C	SER	349	-8.710	-1.287	35.261	1.00	16.03
ATOM	2010	O	SER	349	-9.315	-0.435	35.910	1.00	17.50
ATOM	2011	N	TYR	350	-7.400	-1.466	35.363	1.00	15.01
ATOM	2012	CA	TYR	350	-6.605	-0.645	36.271	1.00	13.82
ATOM	2013	CB	TYR	350	-5.209	-1.257	36.455	1.00	11.61
ATOM	2014	CG	TYR	350	-4.331	-1.216	35.227	1.00	9.92
ATOM	2015	CD1	TYR	350	-3.429	-0.168	35.016	1.00	8.94
ATOM	2016	CE1	TYR	350	-2.608	-0.137	33.890	1.00	9.41
ATOM	2017	CD2	TYR	350	-4.393	-2.228	34.277	1.00	11.27
ATOM	2018	CE2	TYR	350	-3.583	-2.204	33.148	1.00	11.74
ATOM	2019	CZ	TYR	350	-2.691	-1.163	32.958	1.00	11.99
ATOM	2020	OH	TYR	350	-1.880	-1.170	31.843	1.00	14.77
ATOM	2021	C	TYR	350	-6.494	0.791	35.763	1.00	14.36
ATOM	2022	O	TYR	350	-6.070	1.683	36.502	1.00	12.89
ATOM	2023	N	LEU	351	-6.882	1.009	34.504	1.00	11.34
ATOM	2024	CA	LEU	351	-6.834	2.338	33.902	1.00	12.74
ATOM	2025	CB	LEU	351	-6.653	2.231	32.384	1.00	14.15
ATOM	2026	CG	LEU	351	-5.276	1.775	31.894	1.00	16.33
ATOM	2027	CD1	LEU	351	-5.300	1.596	30.378	1.00	15.67
ATOM	2028	CD2	LEU	351	-4.225	2.813	32.294	1.00	14.98
ATOM	2029	C	LEU	351	-8.076	3.169	34.207	1.00	13.96
ATOM	2030	O	LEU	351	-8.096	4.377	33.960	1.00	14.39
ATOM	2031	N	GLN	352	-9.115	2.526	34.728	1.00	15.38
ATOM	2032	CA	GLN	352	-10.340	3.233	35.079	1.00	17.76
ATOM	2033	CB	GLN	352	-11.421	2.251	35.525	1.00	20.66
ATOM	2034	CG	GLN	352	-11.889	1.297	34.446	1.00	24.75
ATOM	2035	CD	GLN	352	-12.793	0.211	34.996	1.00	28.37
ATOM	2036	OE1	GLN	352	-13.384	-0.563	34.241	1.00	29.35
ATOM	2037	NE2	GLN	352	-12.900	0.145	36.321	1.00	28.44
ATOM	2038	C	GLN	352	-10.029	4.196	36.220	1.00	16.75
ATOM	2039	O	GLN	352	-9.304	3.855	37.158	1.00	15.52
ATOM	2040	N	GLN	353	-10.592	5.395	36.128	1.00	16.50
ATOM	2041	CA	GLN	353	-10.394	6.455	37.109	1.00	16.98
ATOM	2042	CB	GLN	353	-11.392	7.574	36.826	1.00	18.43
ATOM	2043	CG	GLN	353	-11.458	8.659	37.869	1.00	20.81
ATOM	2044	CD	GLN	353	-12.396	9.775	37.458	1.00	21.47
ATOM	2045	OE1	GLN	353	-13.542	9.530	37.063	1.00	21.50
ATOM	2046	NE2	GLN	353	-11.916	11.007	37.543	1.00	20.82
ATOM	2047	C	GLN	353	-10.463	6.065	38.587	1.00	15.23
ATOM	2048	O	GLN	353	-9.561	6.402	39.360	1.00	13.51
ATOM	2049	N	GLU	354	-11.519	5.360	38.985	1.00	16.14
ATOM	2050	CA	GLU	354	-11.671	4.980	40.387	1.00	17.49
ATOM	2051	CB	GLU	354	-13.074	4.412	40.658	1.00	20.37
ATOM	2052	CG	GLU	354	-13.410	3.092	39.970	1.00	23.41
ATOM	2053	CD	GLU	354	-13.796	3.260	38.511	1.00	25.49
ATOM	2054	OE1	GLU	354	-14.304	2.282	37.920	1.00	27.89
ATOM	2055	OE2	GLU	354	-13.590	4.361	37.955	1.00	26.10
ATOM	2056	C	GLU	354	-10.618	4.009	40.902	1.00	17.14
ATOM	2057	O	GLU	354	-10.438	3.874	42.114	1.00	18.63
ATOM	2058	N	ALA	355	-9.920	3.328	40.000	1.00	15.68
ATOM	2059	CA	ALA	355	-8.878	2.395	40.427	1.00	13.94
ATOM	2060	CB	ALA	355	-8.892	1.148	39.547	1.00	14.91
ATOM	2061	C	ALA	355	-7.510	3.080	40.351	1.00	13.51
ATOM	2062	O	ALA	355	-6.741	3.081	41.316	1.00	12.42
ATOM	2063	N	TYR	356	-7.225	3.670	39.197	1.00	11.07
ATOM	2064	CA	TYR	356	-5.960	4.357	38.962	1.00	12.96
ATOM	2065	CB	TYR	356	-5.976	4.997	37.575	1.00	10.78
ATOM	2066	CG	TYR	356	-4.607	5.255	37.005	1.00	12.19
ATOM	2067	CD1	TYR	356	-3.895	4.237	36.373	1.00	11.69

ATOM	2068	CE1	TYR	356	-2.640	4.469	35.824	1.00	10.87
ATOM	2069	CD2	TYR	356	-4.025	6.520	37.080	1.00	12.81
ATOM	2070	CE2	TYR	356	-2.769	6.764	36.535	1.00	11.47
ATOM	2071	CZ	TYR	356	-2.084	5.729	35.907	1.00	11.09
ATOM	2072	OH	TYR	356	-0.850	5.955	35.354	1.00	10.60
ATOM	2073	C	TYR	356	-5.648	5.433	40.007	1.00	13.16
ATOM	2074	O	TYR	356	-4.560	5.444	40.581	1.00	12.76
ATOM	2075	N	ASP	357	-6.602	6.331	40.247	1.00	13.84
ATOM	2076	CA	ASP	357	-6.423	7.424	41.204	1.00	18.43
ATOM	2077	CB	ASP	357	-7.581	8.419	41.084	1.00	17.43
ATOM	2078	CG	ASP	357	-7.504	9.246	39.815	1.00	18.38
ATOM	2079	OD1	ASP	357	-6.728	8.869	38.910	1.00	18.08
ATOM	2080	OD2	ASP	357	-8.220	10.268	39.716	1.00	18.42
ATOM	2081	C	ASP	357	-6.274	6.976	42.653	1.00	20.06
ATOM	2082	O	ASP	357	-5.941	7.775	43.528	1.00	23.90
ATOM	2083	N	ARG	358	-6.531	5.702	42.913	1.00	20.44
ATOM	2084	CA	ARG	358	-6.382	5.178	44.257	1.00	21.57
ATOM	2085	CB	ARG	358	-7.560	4.263	44.610	1.00	23.42
ATOM	2086	CG	ARG	358	-7.507	3.723	46.026	1.00	29.08
ATOM	2087	CD	ARG	358	-7.119	2.251	46.063	1.00	32.79
ATOM	2088	NE	ARG	358	-8.268	1.372	45.852	1.00	34.76
ATOM	2089	CZ	ARG	358	-8.226	0.045	45.942	1.00	36.92
ATOM	2090	NH1	ARG	358	-7.087	-0.571	46.234	1.00	37.77
ATOM	2091	NH2	ARG	358	-9.330	-0.668	45.756	1.00	36.07
ATOM	2092	C	ARG	358	-5.075	4.396	44.318	1.00	19.82
ATOM	2093	O	ARG	358	-4.199	4.686	45.138	1.00	18.62
ATOM	2094	N	ASP	359	-4.935	3.428	43.417	1.00	18.33
ATOM	2095	CA	ASP	359	-3.752	2.580	43.381	1.00	18.24
ATOM	2096	CB	ASP	359	-4.033	1.334	42.540	1.00	20.49
ATOM	2097	CG	ASP	359	-5.228	0.548	43.048	1.00	23.10
ATOM	2098	OD1	ASP	359	-5.573	0.684	44.242	1.00	23.12
ATOM	2099	OD2	ASP	359	-5.816	-0.218	42.255	1.00	25.58
ATOM	2100	C	ASP	359	-2.465	3.245	42.890	1.00	18.04
ATOM	2101	O	ASP	359	-1.465	3.254	43.606	1.00	17.47
ATOM	2102	N	PHE	360	-2.480	3.801	41.681	1.00	17.22
ATOM	2103	CA	PHE	360	-1.275	4.426	41.148	1.00	16.82
ATOM	2104	CB	PHE	360	-1.507	4.985	39.743	1.00	16.92
ATOM	2105	CG	PHE	360	-0.237	5.420	39.060	1.00	17.95
ATOM	2106	CD1	PHE	360	0.690	4.476	38.628	1.00	18.65
ATOM	2107	CD2	PHE	360	0.059	6.770	38.903	1.00	16.47
ATOM	2108	CE1	PHE	360	1.900	4.869	38.051	1.00	17.18
ATOM	2109	CE2	PHE	360	1.266	7.179	38.328	1.00	16.88
ATOM	2110	CZ	PHE	360	2.188	6.228	37.902	1.00	18.41
ATOM	2111	C	PHE	360	-0.743	5.539	42.046	1.00	16.12
ATOM	2112	O	PHE	360	0.454	5.595	42.323	1.00	14.27
ATOM	2113	N	LEU	361	-1.627	6.426	42.492	1.00	17.15
ATOM	2114	CA	LEU	361	-1.231	7.534	43.364	1.00	16.51
ATOM	2115	CB	LEU	361	-2.428	8.458	43.634	1.00	18.14
ATOM	2116	CG	LEU	361	-2.845	9.408	42.508	1.00	22.21
ATOM	2117	CD1	LEU	361	-1.675	10.333	42.188	1.00	23.81
ATOM	2118	CD2	LEU	361	-3.257	8.624	41.268	1.00	22.98
ATOM	2119	C	LEU	361	-0.668	7.026	44.688	1.00	15.86
ATOM	2120	O	LEU	361	0.286	7.591	45.232	1.00	14.22
ATOM	2121	N	ALA	362	-1.263	5.960	45.210	1.00	15.49
ATOM	2122	CA	ALA	362	-0.791	5.379	46.461	1.00	15.70
ATOM	2123	CB	ALA	362	-1.735	4.264	46.923	1.00	13.46
ATOM	2124	C	ALA	362	0.604	4.822	46.200	1.00	15.02
ATOM	2125	O	ALA	362	1.507	4.953	47.021	1.00	15.41
ATOM	2126	N	ARG	363	0.769	4.211	45.034	1.00	14.49
ATOM	2127	CA	ARG	363	2.050	3.641	44.640	1.00	14.32
ATOM	2128	CB	ARG	363	1.932	3.021	43.242	1.00	17.08
ATOM	2129	CG	ARG	363	3.121	2.171	42.844	1.00	20.97

ATOM	2130	CD	ARG	363	3.210	1.986	41.331	1.00	20.84
ATOM	2131	NE	ARG	363	4.311	1.094	40.978	1.00	23.25
ATOM	2132	CZ	ARG	363	4.259	-0.233	41.060	1.00	21.83
ATOM	2133	NH1	ARG	363	3.152	-0.833	41.475	1.00	20.51
ATOM	2134	NH2	ARG	363	5.322	-0.959	40.743	1.00	21.73
ATOM	2135	C	ARG	363	3.111	4.745	44.623	1.00	13.49
ATOM	2136	O	ARG	363	4.188	4.597	45.200	1.00	12.63
ATOM	2137	N	VAL	364	2.781	5.855	43.968	1.00	12.59
ATOM	2138	CA	VAL	364	3.677	7.002	43.833	1.00	11.73
ATOM	2139	CB	VAL	364	3.052	8.079	42.905	1.00	10.65
ATOM	2140	CG1	VAL	364	3.893	9.363	42.923	1.00	7.87
ATOM	2141	CG2	VAL	364	2.950	7.542	41.497	1.00	8.51
ATOM	2142	C	VAL	364	4.068	7.658	45.156	1.00	13.57
ATOM	2143	O	VAL	364	5.254	7.887	45.413	1.00	13.39
ATOM	2144	N	TYR	365	3.084	7.973	45.993	1.00	13.68
ATOM	2145	CA	TYR	365	3.390	8.613	47.264	1.00	13.97
ATOM	2146	CB	TYR	365	2.236	9.529	47.685	1.00	14.54
ATOM	2147	CG	TYR	365	2.146	10.750	46.794	1.00	15.61
ATOM	2148	CD1	TYR	365	1.412	10.725	45.607	1.00	16.85
ATOM	2149	CE1	TYR	365	1.410	11.819	44.735	1.00	15.09
ATOM	2150	CD2	TYR	365	2.873	11.899	47.091	1.00	16.88
ATOM	2151	CE2	TYR	365	2.883	12.994	46.229	1.00	14.51
ATOM	2152	CZ	TYR	365	2.153	12.949	45.056	1.00	14.29
ATOM	2153	OH	TYR	365	2.183	14.032	44.204	1.00	12.19
ATOM	2154	C	TYR	365	3.758	7.635	48.371	1.00	14.59
ATOM	2155	O	TYR	365	4.018	8.033	49.511	1.00	16.46
ATOM	2156	N	GLY	366	3.790	6.355	48.019	1.00	14.08
ATOM	2157	CA	GLY	366	4.173	5.325	48.965	1.00	17.80
ATOM	2158	C	GLY	366	5.631	4.979	48.706	1.00	17.99
ATOM	2159	O	GLY	366	6.317	4.415	49.556	1.00	18.47
ATOM	2160	N	ALA	367	6.106	5.332	47.515	1.00	19.12
ATOM	2161	CA	ALA	367	7.486	5.070	47.130	1.00	19.15
ATOM	2162	CB	ALA	367	7.657	5.274	45.628	1.00	19.73
ATOM	2163	C	ALA	367	8.427	5.994	47.895	1.00	19.44
ATOM	2164	O	ALA	367	8.091	7.144	48.181	1.00	18.99
ATOM	2165	N	PRO	368	9.627	5.503	48.230	1.00	19.69
ATOM	2166	CD	PRO	368	10.212	4.190	47.901	1.00	21.23
ATOM	2167	CA	PRO	368	10.583	6.330	48.964	1.00	19.49
ATOM	2168	CB	PRO	368	11.725	5.357	49.249	1.00	19.26
ATOM	2169	CG	PRO	368	11.692	4.453	48.064	1.00	21.55
ATOM	2170	C	PRO	368	11.034	7.552	48.170	1.00	19.99
ATOM	2171	O	PRO	368	11.140	7.511	46.945	1.00	18.43
ATOM	2172	N	GLN	369	11.294	8.643	48.881	1.00	21.41
ATOM	2173	CA	GLN	369	11.743	9.880	48.258	1.00	21.74
ATOM	2174	CB	GLN	369	11.294	11.073	49.102	1.00	22.54
ATOM	2175	CG	GLN	369	11.311	12.401	48.372	1.00	26.16
ATOM	2176	CD	GLN	369	10.619	13.500	49.159	1.00	28.36
ATOM	2177	OE1	GLN	369	9.487	13.330	49.624	1.00	28.27
ATOM	2178	NE2	GLN	369	11.292	14.637	49.307	1.00	27.49
ATOM	2179	C	GLN	369	13.266	9.847	48.166	1.00	21.10
ATOM	2180	O	GLN	369	13.932	9.356	49.075	1.00	20.59
ATOM	2181	N	LEU	370	13.816	10.352	47.067	1.00	21.38
ATOM	2182	CA	LEU	370	15.263	10.366	46.889	1.00	21.26
ATOM	2183	CB	LEU	370	15.703	9.184	46.010	1.00	20.85
ATOM	2184	CG	LEU	370	17.209	8.906	45.916	1.00	18.68
ATOM	2185	CD1	LEU	370	17.738	8.511	47.293	1.00	19.19
ATOM	2186	CD2	LEU	370	17.480	7.795	44.910	1.00	19.97
ATOM	2187	C	LEU	370	15.726	11.680	46.262	1.00	21.87
ATOM	2188	O	LEU	370	15.071	12.223	45.366	1.00	21.38
ATOM	2189	N	GLN	371	16.853	12.193	46.749	1.00	21.98
ATOM	2190	CA	GLN	371	17.421	13.435	46.236	1.00	22.20
ATOM	2191	CB	GLN	371	18.704	13.772	46.996	1.00	24.96

ATOM	2192	CG	GLN	371	18.466	14.277	48.404	1.00	30.20
ATOM	2193	CD	GLN	371	19.611	13.954	49.338	1.00	34.30
ATOM	2194	OE1	GLN	371	20.779	14.178	49.012	1.00	37.08
ATOM	2195	NE2	GLN	371	19.284	13.425	50.514	1.00	35.32
ATOM	2196	C	GLN	371	17.724	13.271	44.754	1.00	21.55
ATOM	2197	O	GLN	371	18.327	12.281	44.348	1.00	19.64
ATOM	2198	N	VAL	372	17.310	14.243	43.948	1.00	20.33
ATOM	2199	CA	VAL	372	17.538	14.174	42.509	1.00	20.92
ATOM	2200	CB	VAL	372	17.175	15.520	41.825	1.00	20.80
ATOM	2201	CG1	VAL	372	18.057	16.638	42.355	1.00	20.88
ATOM	2202	CG2	VAL	372	17.303	15.388	40.315	1.00	17.69
ATOM	2203	C	VAL	372	18.979	13.791	42.162	1.00	21.73
ATOM	2204	O	VAL	372	19.218	12.952	41.291	1.00	21.87
ATOM	2205	N	GLU	373	19.936	14.393	42.861	1.00	22.76
ATOM	2206	CA	GLU	373	21.349	14.122	42.625	1.00	23.19
ATOM	2207	CB	GLU	373	22.203	14.986	43.559	1.00	26.24
ATOM	2208	CG	GLU	373	23.694	14.976	43.259	1.00	31.34
ATOM	2209	CD	GLU	373	24.015	15.469	41.857	1.00	34.33
ATOM	2210	OE1	GLU	373	23.434	16.494	41.436	1.00	35.35
ATOM	2211	OE2	GLU	373	24.855	14.836	41.180	1.00	34.92
ATOM	2212	C	GLU	373	21.677	12.644	42.837	1.00	21.78
ATOM	2213	O	GLU	373	22.488	12.070	42.114	1.00	18.08
ATOM	2214	N	LYS	374	21.053	12.029	43.837	1.00	19.84
ATOM	2215	CA	LYS	374	21.297	10.620	44.105	1.00	20.12
ATOM	2216	CB	LYS	374	20.638	10.214	45.426	1.00	20.76
ATOM	2217	CG	LYS	374	21.292	10.847	46.645	1.00	22.75
ATOM	2218	CD	LYS	374	20.684	10.334	47.938	1.00	24.93
ATOM	2219	CE	LYS	374	21.393	10.925	49.144	1.00	27.91
ATOM	2220	NZ	LYS	374	20.832	10.403	50.427	1.00	29.95
ATOM	2221	C	LYS	374	20.783	9.752	42.954	1.00	19.88
ATOM	2222	O	LYS	374	21.390	8.730	42.612	1.00	19.12
ATOM	2223	N	VAL	375	19.674	10.167	42.349	1.00	18.37
ATOM	2224	CA	VAL	375	19.096	9.427	41.233	1.00	19.39
ATOM	2225	CB	VAL	375	17.686	9.958	40.867	1.00	18.97
ATOM	2226	CG1	VAL	375	17.134	9.187	39.672	1.00	18.94
ATOM	2227	CG2	VAL	375	16.750	9.832	42.056	1.00	16.98
ATOM	2228	C	VAL	375	19.987	9.559	40.000	1.00	21.63
ATOM	2229	O	VAL	375	20.326	8.566	39.358	1.00	21.10
ATOM	2230	N	ARG	376	20.362	10.795	39.683	1.00	23.12
ATOM	2231	CA	ARG	376	21.197	11.084	38.523	1.00	26.09
ATOM	2232	CB	ARG	376	21.539	12.580	38.464	1.00	27.23
ATOM	2233	CG	ARG	376	22.178	12.985	37.138	1.00	31.52
ATOM	2234	CD	ARG	376	23.052	14.233	37.227	1.00	34.56
ATOM	2235	NE	ARG	376	22.297	15.472	37.392	1.00	36.77
ATOM	2236	CZ	ARG	376	22.821	16.685	37.229	1.00	38.78
ATOM	2237	NH1	ARG	376	24.098	16.818	36.895	1.00	39.71
ATOM	2238	NH2	ARG	376	22.075	17.769	37.403	1.00	39.07
ATOM	2239	C	ARG	376	22.493	10.276	38.501	1.00	25.31
ATOM	2240	O	ARG	376	22.886	9.755	37.458	1.00	26.40
ATOM	2241	N	THR	377	23.151	10.166	39.652	1.00	26.37
ATOM	2242	CA	THR	377	24.414	9.437	39.739	1.00	26.63
ATOM	2243	CB	THR	377	25.329	10.045	40.806	1.00	26.36
ATOM	2244	OG1	THR	377	24.726	9.886	42.096	1.00	26.44
ATOM	2245	CG2	THR	377	25.548	11.524	40.528	1.00	27.30
ATOM	2246	C	THR	377	24.254	7.955	40.051	1.00	26.23
ATOM	2247	O	THR	377	25.240	7.257	40.281	1.00	27.46
ATOM	2248	N	ASN	378	23.014	7.480	40.068	1.00	25.76
ATOM	2249	CA	ASN	378	22.731	6.074	40.339	1.00	25.02
ATOM	2250	CB	ASN	378	23.445	5.184	39.317	1.00	26.09
ATOM	2251	CG	ASN	378	22.498	4.245	38.597	1.00	26.44
ATOM	2252	OD1	ASN	378	21.617	3.642	39.210	1.00	26.28
ATOM	2253	ND2	ASN	378	22.683	4.107	37.289	1.00	28.85

ATOM	2254	C	ASN	378	23.119	5.625	41.749	1.00	24.81
ATOM	2255	O	ASN	378	23.613	4.511	41.938	1.00	24.28
ATOM	2256	N	ASP	379	22.900	6.485	42.738	1.00	24.43
ATOM	2257	CA	ASP	379	23.215	6.133	44.118	1.00	25.28
ATOM	2258	CB	ASP	379	23.579	7.387	44.916	1.00	27.76
ATOM	2259	CG	ASP	379	23.936	7.076	46.356	1.00	30.86
ATOM	2260	OD1	ASP	379	24.767	6.170	46.579	1.00	30.08
ATOM	2261	OD2	ASP	379	23.391	7.740	47.265	1.00	34.52
ATOM	2262	C	ASP	379	21.997	5.444	44.740	1.00	24.84
ATOM	2263	O	ASP	379	20.873	5.596	44.249	1.00	25.18
ATOM	2264	N	ARG	380	22.220	4.677	45.806	1.00	22.13
ATOM	2265	CA	ARG	380	21.131	3.976	46.480	1.00	20.43
ATOM	2266	CB	ARG	380	20.206	4.988	47.160	1.00	20.12
ATOM	2267	CG	ARG	380	20.855	5.802	48.270	1.00	20.68
ATOM	2268	CD	ARG	380	21.123	4.952	49.501	1.00	21.18
ATOM	2269	NE	ARG	380	19.889	4.420	50.077	1.00	21.63
ATOM	2270	CZ	ARG	380	18.930	5.171	50.611	1.00	22.90
ATOM	2271	NH1	ARG	380	19.061	6.489	50.647	1.00	21.89
ATOM	2272	NH2	ARG	380	17.835	4.605	51.105	1.00	24.01
ATOM	2273	C	ARG	380	20.324	3.128	45.494	1.00	19.34
ATOM	2274	O	ARG	380	19.098	3.213	45.447	1.00	19.29
ATOM	2275	N	LYS	381	21.012	2.297	44.720	1.00	18.25
ATOM	2276	CA	LYS	381	20.345	1.464	43.727	1.00	18.48
ATOM	2277	CB	LYS	381	21.394	0.782	42.842	1.00	20.79
ATOM	2278	CG	LYS	381	22.205	1.773	42.020	1.00	23.49
ATOM	2279	CD	LYS	381	23.453	1.154	41.407	1.00	26.11
ATOM	2280	CE	LYS	381	23.120	0.111	40.358	1.00	26.77
ATOM	2281	NZ	LYS	381	24.361	-0.373	39.685	1.00	30.23
ATOM	2282	C	LYS	381	19.371	0.429	44.286	1.00	16.54
ATOM	2283	O	LYS	381	18.585	-0.143	43.533	1.00	14.84
ATOM	2284	N	GLU	382	19.401	0.188	45.594	1.00	15.66
ATOM	2285	CA	GLU	382	18.484	-0.787	46.174	1.00	13.79
ATOM	2286	CB	GLU	382	18.804	-1.062	47.652	1.00	14.52
ATOM	2287	CG	GLU	382	18.574	0.125	48.573	1.00	14.59
ATOM	2288	CD	GLU	382	19.790	1.011	48.688	1.00	12.70
ATOM	2289	OE1	GLU	382	20.591	1.046	47.729	1.00	13.35
ATOM	2290	OE2	GLU	382	19.941	1.679	49.734	1.00	13.65
ATOM	2291	C	GLU	382	17.058	-0.265	46.061	1.00	15.15
ATOM	2292	O	GLU	382	16.100	-1.013	46.250	1.00	14.00
ATOM	2293	N	LEU	383	16.924	1.025	45.757	1.00	14.56
ATOM	2294	CA	LEU	383	15.612	1.650	45.615	1.00	14.11
ATOM	2295	CB	LEU	383	15.664	3.102	46.109	1.00	12.18
ATOM	2296	CG	LEU	383	16.181	3.286	47.541	1.00	13.12
ATOM	2297	CD1	LEU	383	16.328	4.768	47.874	1.00	11.23
ATOM	2298	CD2	LEU	383	15.224	2.599	48.516	1.00	14.16
ATOM	2299	C	LEU	383	15.210	1.601	44.142	1.00	15.08
ATOM	2300	O	LEU	383	15.468	2.539	43.390	1.00	16.65
ATOM	2301	N	GLY	384	14.591	0.493	43.742	1.00	14.70
ATOM	2302	CA	GLY	384	14.170	0.316	42.362	1.00	15.11
ATOM	2303	C	GLY	384	13.067	1.250	41.889	1.00	15.48
ATOM	2304	O	GLY	384	12.846	1.389	40.682	1.00	15.95
ATOM	2305	N	GLU	385	12.369	1.888	42.823	1.00	14.39
ATOM	2306	CA	GLU	385	11.292	2.813	42.463	1.00	12.78
ATOM	2307	CB	GLU	385	9.933	2.097	42.485	1.00	12.38
ATOM	2308	CG	GLU	385	8.782	2.939	41.934	1.00	13.09
ATOM	2309	CD	GLU	385	7.536	2.115	41.640	1.00	13.56
ATOM	2310	OE1	GLU	385	7.657	0.880	41.525	1.00	13.77
ATOM	2311	OE2	GLU	385	6.439	2.698	41.511	1.00	12.40
ATOM	2312	C	GLU	385	11.286	3.974	43.444	1.00	12.89
ATOM	2313	O	GLU	385	11.017	3.799	44.635	1.00	13.97
ATOM	2314	N	VAL	386	11.583	5.167	42.944	1.00	10.84
ATOM	2315	CA	VAL	386	11.625	6.331	43.811	1.00	11.04

ATOM	2316	CB	VAL	386	13.057	6.850	43.970	1.00	11.92
ATOM	2317	CG1	VAL	386	13.952	5.754	44.524	1.00	12.59
ATOM	2318	CG2	VAL	386	13.574	7.353	42.623	1.00	9.11
ATOM	2319	C	VAL	386	10.775	7.489	43.339	1.00	12.41
ATOM	2320	O	VAL	386	10.228	7.491	42.228	1.00	11.29
ATOM	2321	N	ARG	387	10.689	8.484	44.207	1.00	13.26
ATOM	2322	CA	ARG	387	9.939	9.691	43.947	1.00	15.32
ATOM	2323	CB	ARG	387	8.752	9.773	44.913	1.00	16.94
ATOM	2324	CG	ARG	387	7.966	11.067	44.878	1.00	17.77
ATOM	2325	CD	ARG	387	6.596	10.863	45.513	1.00	18.00
ATOM	2326	NE	ARG	387	6.678	10.183	46.806	1.00	23.24
ATOM	2327	CZ	ARG	387	7.030	10.770	47.947	1.00	23.22
ATOM	2328	NH1	ARG	387	7.334	12.059	47.967	1.00	24.56
ATOM	2329	NH2	ARG	387	7.076	10.067	49.071	1.00	22.83
ATOM	2330	C	ARG	387	10.862	10.882	44.147	1.00	16.39
ATOM	2331	O	ARG	387	11.411	11.071	45.228	1.00	18.64
ATOM	2332	N	VAL	388	11.068	11.652	43.085	1.00	16.66
ATOM	2333	CA	VAL	388	11.886	12.857	43.153	1.00	15.67
ATOM	2334	CB	VAL	388	12.742	13.052	41.881	1.00	16.98
ATOM	2335	CG1	VAL	388	13.402	14.436	41.899	1.00	17.19
ATOM	2336	CG2	VAL	388	13.816	11.970	41.808	1.00	15.77
ATOM	2337	C	VAL	388	10.846	13.963	43.254	1.00	17.25
ATOM	2338	O	VAL	388	10.094	14.212	42.310	1.00	15.87
ATOM	2339	N	GLN	389	10.791	14.612	44.409	1.00	16.54
ATOM	2340	CA	GLN	389	9.800	15.657	44.639	1.00	18.22
ATOM	2341	CB	GLN	389	9.389	15.657	46.116	1.00	19.02
ATOM	2342	CG	GLN	389	8.448	16.788	46.520	1.00	21.90
ATOM	2343	CD	GLN	389	7.931	16.637	47.945	1.00	22.72
ATOM	2344	OE1	GLN	389	7.150	15.731	48.242	1.00	24.17
ATOM	2345	NE2	GLN	389	8.371	17.522	48.834	1.00	23.18
ATOM	2346	C	GLN	389	10.250	17.048	44.235	1.00	17.31
ATOM	2347	O	GLN	389	11.360	17.468	44.557	1.00	17.38
ATOM	2348	N	TYR	390	9.384	17.748	43.508	1.00	16.61
ATOM	2349	CA	TYR	390	9.660	19.117	43.091	1.00	17.60
ATOM	2350	CB	TYR	390	9.576	19.257	41.561	1.00	16.03
ATOM	2351	CG	TYR	390	8.199	19.058	40.951	1.00	14.48
ATOM	2352	CD1	TYR	390	7.253	20.091	40.953	1.00	13.47
ATOM	2353	CE1	TYR	390	6.007	19.934	40.344	1.00	14.26
ATOM	2354	CD2	TYR	390	7.859	17.856	40.329	1.00	13.94
ATOM	2355	CE2	TYR	390	6.613	17.684	39.715	1.00	13.51
ATOM	2356	CZ	TYR	390	5.694	18.727	39.723	1.00	15.18
ATOM	2357	OH	TYR	390	4.479	18.574	39.090	1.00	10.32
ATOM	2358	C	TYR	390	8.596	19.960	43.789	1.00	18.34
ATOM	2359	O	TYR	390	7.476	19.494	44.007	1.00	17.98
ATOM	2360	N	THR	391	8.941	21.185	44.157	1.00	18.74
ATOM	2361	CA	THR	391	7.995	22.042	44.859	1.00	21.58
ATOM	2362	CB	THR	391	8.576	22.501	46.210	1.00	20.80
ATOM	2363	OG1	THR	391	9.866	23.083	45.998	1.00	20.85
ATOM	2364	CG2	THR	391	8.708	21.322	47.158	1.00	22.12
ATOM	2365	C	THR	391	7.570	23.270	44.071	1.00	22.88
ATOM	2366	O	THR	391	6.434	23.720	44.177	1.00	26.11
ATOM	2367	N	GLY	392	8.481	23.820	43.282	1.00	23.52
ATOM	2368	CA	GLY	392	8.135	24.994	42.507	1.00	24.22
ATOM	2369	C	GLY	392	8.413	24.806	41.036	1.00	23.77
ATOM	2370	O	GLY	392	8.889	23.754	40.613	1.00	22.59
ATOM	2371	N	ARG	393	8.112	25.831	40.252	1.00	24.05
ATOM	2372	CA	ARG	393	8.340	25.782	38.817	1.00	25.79
ATOM	2373	CB	ARG	393	7.764	27.040	38.161	1.00	28.38
ATOM	2374	CG	ARG	393	8.209	28.349	38.805	1.00	32.75
ATOM	2375	CD	ARG	393	7.385	29.523	38.291	1.00	33.47
ATOM	2376	NE	ARG	393	6.011	29.495	38.788	1.00	37.05
ATOM	2377	CZ	ARG	393	5.024	30.247	38.305	1.00	38.07

ATOM	2378	NH1	ARG	393	5.262	31.086	37.307	1.00	38.83
ATOM	2379	NH2	ARG	393	3.801	30.163	38.817	1.00	35.69
ATOM	2380	C	ARG	393	9.830	25.645	38.509	1.00	24.14
ATOM	2381	O	ARG	393	10.213	24.932	37.587	1.00	24.42
ATOM	2382	N	ASP	394	10.667	26.322	39.290	1.00	25.09
ATOM	2383	CA	ASP	394	12.113	26.259	39.091	1.00	24.07
ATOM	2384	CB	ASP	394	12.827	27.262	40.003	1.00	26.58
ATOM	2385	CG	ASP	394	12.520	28.699	39.642	1.00	29.74
ATOM	2386	OD1	ASP	394	12.645	29.047	38.450	1.00	33.04
ATOM	2387	OD2	ASP	394	12.161	29.483	40.548	1.00	31.55
ATOM	2388	C	ASP	394	12.665	24.861	39.359	1.00	22.25
ATOM	2389	O	ASP	394	13.485	24.353	38.590	1.00	19.78
ATOM	2390	N	SER	395	12.227	24.246	40.456	1.00	19.30
ATOM	2391	CA	SER	395	12.692	22.909	40.796	1.00	19.96
ATOM	2392	CB	SER	395	12.238	22.512	42.211	1.00	20.52
ATOM	2393	OG	SER	395	10.830	22.598	42.371	1.00	24.11
ATOM	2394	C	SER	395	12.204	21.886	39.768	1.00	19.37
ATOM	2395	O	SER	395	12.943	20.967	39.401	1.00	17.06
ATOM	2396	N	PHE	396	10.970	22.039	39.293	1.00	17.87
ATOM	2397	CA	PHE	396	10.455	21.105	38.295	1.00	18.41
ATOM	2398	CB	PHE	396	9.037	21.476	37.848	1.00	17.34
ATOM	2399	CG	PHE	396	8.585	20.723	36.627	1.00	18.05
ATOM	2400	CD1	PHE	396	8.241	19.375	36.710	1.00	17.79
ATOM	2401	CD2	PHE	396	8.584	21.337	35.378	1.00	17.15
ATOM	2402	CE1	PHE	396	7.910	18.649	35.568	1.00	16.33
ATOM	2403	CE2	PHE	396	8.255	20.618	34.231	1.00	17.41
ATOM	2404	CZ	PHE	396	7.919	19.271	34.327	1.00	15.40
ATOM	2405	C	PHE	396	11.353	21.090	37.064	1.00	18.07
ATOM	2406	O	PHE	396	11.840	20.037	36.650	1.00	17.79
ATOM	2407	N	LYS	397	11.571	22.264	36.478	1.00	18.12
ATOM	2408	CA	LYS	397	12.398	22.368	35.281	1.00	21.40
ATOM	2409	CB	LYS	397	12.375	23.802	34.743	1.00	22.74
ATOM	2410	CG	LYS	397	11.196	24.077	33.808	1.00	24.43
ATOM	2411	CD	LYS	397	11.178	25.516	33.334	1.00	26.07
ATOM	2412	CE	LYS	397	10.153	25.709	32.230	1.00	28.64
ATOM	2413	NZ	LYS	397	10.497	24.888	31.031	1.00	30.72
ATOM	2414	C	LYS	397	13.837	21.906	35.470	1.00	21.01
ATOM	2415	O	LYS	397	14.429	21.326	34.561	1.00	21.83
ATOM	2416	N	ALA	398	14.401	22.158	36.645	1.00	21.60
ATOM	2417	CA	ALA	398	15.775	21.750	36.917	1.00	21.24
ATOM	2418	CB	ALA	398	16.263	22.391	38.203	1.00	20.78
ATOM	2419	C	ALA	398	15.872	20.231	37.017	1.00	20.78
ATOM	2420	O	ALA	398	16.692	19.607	36.346	1.00	21.75
ATOM	2421	N	PHE	399	15.025	19.638	37.852	1.00	20.96
ATOM	2422	CA	PHE	399	15.029	18.192	38.035	1.00	19.99
ATOM	2423	CB	PHE	399	14.028	17.797	39.125	1.00	18.54
ATOM	2424	CG	PHE	399	14.339	18.379	40.486	1.00	17.05
ATOM	2425	CD1	PHE	399	13.482	18.157	41.557	1.00	16.31
ATOM	2426	CD2	PHE	399	15.482	19.152	40.693	1.00	15.91
ATOM	2427	CE1	PHE	399	13.753	18.694	42.823	1.00	17.56
ATOM	2428	CE2	PHE	399	15.765	19.692	41.946	1.00	14.25
ATOM	2429	CZ	PHE	399	14.897	19.463	43.016	1.00	16.10
ATOM	2430	C	PHE	399	14.700	17.473	36.725	1.00	21.51
ATOM	2431	O	PHE	399	15.347	16.483	36.374	1.00	22.04
ATOM	2432	N	ALA	400	13.701	17.979	36.003	1.00	20.82
ATOM	2433	CA	ALA	400	13.294	17.392	34.729	1.00	20.91
ATOM	2434	CB	ALA	400	12.141	18.197	34.130	1.00	19.73
ATOM	2435	C	ALA	400	14.470	17.365	33.754	1.00	21.20
ATOM	2436	O	ALA	400	14.773	16.337	33.149	1.00	20.89
ATOM	2437	N	LYS	401	15.124	18.510	33.608	1.00	21.62
ATOM	2438	CA	LYS	401	16.265	18.639	32.715	1.00	23.05
ATOM	2439	CB	LYS	401	16.671	20.115	32.628	1.00	24.94

ATOM	2440	CG	LYS	401	17.885	20.409	31.766	1.00	28.17
ATOM	2441	CD	LYS	401	18.061	21.918	31.609	1.00	30.73
ATOM	2442	CE	LYS	401	19.456	22.276	31.123	1.00	32.62
ATOM	2443	NZ	LYS	401	20.493	21.907	32.131	1.00	32.62
ATOM	2444	C	LYS	401	17.434	17.783	33.210	1.00	22.04
ATOM	2445	O	LYS	401	18.190	17.227	32.417	1.00	23.76
ATOM	2446	N	ALA	402	17.570	17.664	34.524	1.00	22.28
ATOM	2447	CA	ALA	402	18.649	16.874	35.099	1.00	20.76
ATOM	2448	CB	ALA	402	18.726	17.118	36.599	1.00	21.02
ATOM	2449	C	ALA	402	18.484	15.379	34.820	1.00	21.33
ATOM	2450	O	ALA	402	19.472	14.653	34.709	1.00	20.68
ATOM	2451	N	LEU	403	17.240	14.924	34.698	1.00	20.61
ATOM	2452	CA	LEU	403	16.971	13.509	34.449	1.00	22.11
ATOM	2453	CB	LEU	403	15.851	13.023	35.373	1.00	21.57
ATOM	2454	CG	LEU	403	16.123	13.226	36.866	1.00	23.28
ATOM	2455	CD1	LEU	403	14.888	12.874	37.668	1.00	23.31
ATOM	2456	CD2	LEU	403	17.310	12.377	37.297	1.00	23.18
ATOM	2457	C	LEU	403	16.625	13.181	32.994	1.00	21.72
ATOM	2458	O	LEU	403	16.333	12.031	32.667	1.00	22.64
ATOM	2459	N	GLY	404	16.649	14.189	32.127	1.00	20.93
ATOM	2460	CA	GLY	404	16.372	13.958	30.719	1.00	20.37
ATOM	2461	C	GLY	404	14.918	13.926	30.281	1.00	19.89
ATOM	2462	O	GLY	404	14.607	13.409	29.206	1.00	17.75
ATOM	2463	N	VAL	405	14.029	14.473	31.104	1.00	20.35
ATOM	2464	CA	VAL	405	12.606	14.517	30.784	1.00	20.28
ATOM	2465	CB	VAL	405	11.743	14.505	32.072	1.00	21.57
ATOM	2466	CG1	VAL	405	10.275	14.711	31.720	1.00	22.66
ATOM	2467	CG2	VAL	405	11.929	13.194	32.814	1.00	21.79
ATOM	2468	C	VAL	405	12.312	15.806	30.018	1.00	20.54
ATOM	2469	O	VAL	405	12.971	16.825	30.243	1.00	18.46
ATOM	2470	N	MET	406	11.344	15.765	29.105	1.00	20.02
ATOM	2471	CA	MET	406	10.992	16.968	28.357	1.00	22.08
ATOM	2472	CB	MET	406	9.880	16.671	27.340	1.00	23.50
ATOM	2473	CG	MET	406	9.566	17.829	26.383	1.00	27.75
ATOM	2474	SD	MET	406	11.016	18.521	25.531	1.00	28.78
ATOM	2475	CE	MET	406	11.243	20.047	26.440	1.00	30.06
ATOM	2476	C	MET	406	10.518	17.932	29.438	1.00	21.76
ATOM	2477	O	MET	406	9.653	17.589	30.241	1.00	21.41
ATOM	2478	N	ASP	407	11.096	19.129	29.467	1.00	21.77
ATOM	2479	CA	ASP	407	10.771	20.100	30.505	1.00	21.08
ATOM	2480	CB	ASP	407	12.076	20.685	31.063	1.00	22.38
ATOM	2481	CG	ASP	407	12.946	21.318	29.989	1.00	22.76
ATOM	2482	OD1	ASP	407	12.736	21.033	28.792	1.00	21.57
ATOM	2483	OD2	ASP	407	13.857	22.095	30.347	1.00	24.90
ATOM	2484	C	ASP	407	9.799	21.237	30.203	1.00	19.96
ATOM	2485	O	ASP	407	9.506	22.035	31.093	1.00	20.55
ATOM	2486	N	ASP	408	9.289	21.328	28.979	1.00	17.20
ATOM	2487	CA	ASP	408	8.355	22.408	28.663	1.00	16.72
ATOM	2488	CB	ASP	408	8.241	22.597	27.139	1.00	16.96
ATOM	2489	CG	ASP	408	7.546	21.436	26.443	1.00	19.28
ATOM	2490	OD1	ASP	408	7.844	20.267	26.774	1.00	22.15
ATOM	2491	OD2	ASP	408	6.713	21.695	25.547	1.00	17.92
ATOM	2492	C	ASP	408	6.991	22.100	29.278	1.00	16.53
ATOM	2493	O	ASP	408	6.742	20.967	29.698	1.00	15.68
ATOM	2494	N	LEU	409	6.123	23.108	29.358	1.00	13.75
ATOM	2495	CA	LEU	409	4.791	22.921	29.929	1.00	13.61
ATOM	2496	CB	LEU	409	4.738	23.494	31.350	1.00	13.38
ATOM	2497	CG	LEU	409	5.663	22.872	32.401	1.00	13.92
ATOM	2498	CD1	LEU	409	6.723	23.884	32.808	1.00	12.14
ATOM	2499	CD2	LEU	409	4.850	22.434	33.608	1.00	12.33
ATOM	2500	C	LEU	409	3.688	23.574	29.088	1.00	14.06
ATOM	2501	O	LEU	409	3.868	24.670	28.557	1.00	16.08

ATOM	2502	N	LYS	410	2.544	22.901	28.971	1.00	12.50
ATOM	2503	CA	LYS	410	1.417	23.448	28.214	1.00	10.63
ATOM	2504	CB	LYS	410	0.999	22.493	27.092	1.00	11.27
ATOM	2505	CG	LYS	410	2.092	22.191	26.060	1.00	10.21
ATOM	2506	CD	LYS	410	2.481	23.416	25.244	1.00	11.66
ATOM	2507	CE	LYS	410	3.376	23.020	24.069	1.00	13.61
ATOM	2508	NZ	LYS	410	3.712	24.168	23.166	1.00	17.09
ATOM	2509	C	LYS	410	0.260	23.665	29.187	1.00	9.76
ATOM	2510	O	LYS	410	-0.248	22.715	29.785	1.00	9.77
ATOM	2511	N	SER	411	-0.159	24.918	29.339	1.00	8.73
ATOM	2512	CA	SER	411	-1.226	25.262	30.275	1.00	8.95
ATOM	2513	CB	SER	411	-2.566	24.675	29.826	1.00	8.15
ATOM	2514	OG	SER	411	-3.062	25.372	28.695	1.00	9.10
ATOM	2515	C	SER	411	-0.875	24.759	31.669	1.00	9.74
ATOM	2516	O	SER	411	-1.753	24.371	32.443	1.00	8.24
ATOM	2517	N	GLY	412	0.420	24.761	31.978	1.00	8.09
ATOM	2518	CA	GLY	412	0.872	24.327	33.291	1.00	10.26
ATOM	2519	C	GLY	412	1.100	22.832	33.451	1.00	11.79
ATOM	2520	O	GLY	412	1.639	22.397	34.462	1.00	12.61
ATOM	2521	N	VAL	413	0.704	22.047	32.453	1.00	10.75
ATOM	2522	CA	VAL	413	0.853	20.591	32.511	1.00	11.06
ATOM	2523	CB	VAL	413	-0.324	19.888	31.795	1.00	10.00
ATOM	2524	CG1	VAL	413	-0.202	18.363	31.945	1.00	7.62
ATOM	2525	CG2	VAL	413	-1.648	20.394	32.355	1.00	7.68
ATOM	2526	C	VAL	413	2.144	20.068	31.887	1.00	11.55
ATOM	2527	O	VAL	413	2.450	20.364	30.730	1.00	13.14
ATOM	2528	N	PRO	414	2.920	19.280	32.649	1.00	12.70
ATOM	2529	CD	PRO	414	2.823	19.074	34.105	1.00	12.67
ATOM	2530	CA	PRO	414	4.175	18.724	32.131	1.00	13.33
ATOM	2531	CB	PRO	414	4.915	18.306	33.399	1.00	13.45
ATOM	2532	CG	PRO	414	3.804	17.956	34.334	1.00	14.46
ATOM	2533	C	PRO	414	3.952	17.550	31.177	1.00	12.90
ATOM	2534	O	PRO	414	2.885	16.929	31.168	1.00	12.31
ATOM	2535	N	ARG	415	4.971	17.259	30.378	1.00	12.74
ATOM	2536	CA	ARG	415	4.935	16.172	29.409	1.00	12.24
ATOM	2537	CB	ARG	415	6.280	16.097	28.686	1.00	14.24
ATOM	2538	CG	ARG	415	6.575	17.295	27.812	1.00	13.29
ATOM	2539	CD	ARG	415	5.984	17.117	26.426	1.00	14.14
ATOM	2540	NE	ARG	415	6.062	18.343	25.640	1.00	14.15
ATOM	2541	CZ	ARG	415	5.623	18.458	24.391	1.00	15.70
ATOM	2542	NH1	ARG	415	5.075	17.414	23.778	1.00	14.54
ATOM	2543	NH2	ARG	415	5.723	19.620	23.760	1.00	14.77
ATOM	2544	C	ARG	415	4.647	14.838	30.087	1.00	10.04
ATOM	2545	O	ARG	415	5.378	14.429	30.988	1.00	7.92
ATOM	2546	N	ALA	416	3.580	14.173	29.648	1.00	10.43
ATOM	2547	CA	ALA	416	3.162	12.877	30.189	1.00	8.58
ATOM	2548	CB	ALA	416	4.262	11.831	29.967	1.00	9.60
ATOM	2549	C	ALA	416	2.796	12.941	31.670	1.00	11.11
ATOM	2550	O	ALA	416	2.717	11.913	32.348	1.00	11.51
ATOM	2551	N	GLY	417	2.561	14.146	32.170	1.00	9.81
ATOM	2552	CA	GLY	417	2.214	14.292	33.572	1.00	10.51
ATOM	2553	C	GLY	417	0.782	13.926	33.911	1.00	10.46
ATOM	2554	O	GLY	417	-0.124	14.046	33.083	1.00	8.59
ATOM	2555	N	TYR	418	0.587	13.458	35.138	1.00	11.15
ATOM	2556	CA	TYR	418	-0.731	13.096	35.645	1.00	10.88
ATOM	2557	CB	TYR	418	-0.958	11.585	35.589	1.00	12.01
ATOM	2558	CG	TYR	418	-2.381	11.216	35.917	1.00	12.24
ATOM	2559	CD1	TYR	418	-3.424	11.579	35.067	1.00	13.07
ATOM	2560	CE1	TYR	418	-4.749	11.277	35.383	1.00	13.73
ATOM	2561	CD2	TYR	418	-2.694	10.540	37.095	1.00	12.84
ATOM	2562	CE2	TYR	418	-4.014	10.235	37.422	1.00	14.94
ATOM	2563	CZ	TYR	418	-5.033	10.606	36.561	1.00	14.53

ATOM	2564	OH	TYR	418	-6.336	10.301	36.872	1.00	13.70
ATOM	2565	C	TYR	418	-0.736	13.563	37.094	1.00	11.32
ATOM	2566	O	TYR	418	0.067	13.096	37.896	1.00	11.27
ATOM	2567	N	ARG	419	-1.646	14.477	37.425	1.00	11.69
ATOM	2568	CA	ARG	419	-1.713	15.056	38.762	1.00	10.66
ATOM	2569	CB	ARG	419	-2.143	14.019	39.804	1.00	12.58
ATOM	2570	CG	ARG	419	-3.562	13.486	39.589	1.00	14.36
ATOM	2571	CD	ARG	419	-4.071	12.744	40.813	1.00	16.64
ATOM	2572	NE	ARG	419	-4.251	13.635	41.959	1.00	17.62
ATOM	2573	CZ	ARG	419	-5.274	14.473	42.104	1.00	18.66
ATOM	2574	NH1	ARG	419	-6.221	14.537	41.177	1.00	16.30
ATOM	2575	NH2	ARG	419	-5.350	15.254	43.175	1.00	18.36
ATOM	2576	C	ARG	419	-0.320	15.598	39.071	1.00	12.17
ATOM	2577	O	ARG	419	0.155	15.547	40.212	1.00	12.09
ATOM	2578	N	GLY	420	0.323	16.104	38.019	1.00	9.51
ATOM	2579	CA	GLY	420	1.653	16.688	38.115	1.00	10.98
ATOM	2580	C	GLY	420	2.801	15.692	38.095	1.00	10.47
ATOM	2581	O	GLY	420	3.965	16.073	37.996	1.00	11.94
ATOM	2582	N	ILE	421	2.467	14.411	38.165	1.00	10.80
ATOM	2583	CA	ILE	421	3.466	13.350	38.205	1.00	9.69
ATOM	2584	CB	ILE	421	2.904	12.129	38.961	1.00	11.23
ATOM	2585	CG2	ILE	421	3.977	11.060	39.110	1.00	8.27
ATOM	2586	CG1	ILE	421	2.375	12.569	40.327	1.00	9.35
ATOM	2587	CD1	ILE	421	1.393	11.589	40.937	1.00	8.73
ATOM	2588	C	ILE	421	3.972	12.869	36.853	1.00	10.49
ATOM	2589	O	ILE	421	3.193	12.426	36.008	1.00	8.12
ATOM	2590	N	VAL	422	5.285	12.954	36.657	1.00	10.12
ATOM	2591	CA	VAL	422	5.911	12.487	35.427	1.00	10.09
ATOM	2592	CB	VAL	422	6.924	13.514	34.872	1.00	8.63
ATOM	2593	CG1	VAL	422	7.551	12.987	33.577	1.00	8.32
ATOM	2594	CG2	VAL	422	6.219	14.832	34.604	1.00	5.42
ATOM	2595	C	VAL	422	6.631	11.188	35.787	1.00	11.35
ATOM	2596	O	VAL	422	7.531	11.179	36.638	1.00	11.87
ATOM	2597	N	THR	423	6.217	10.095	35.149	1.00	12.70
ATOM	2598	CA	THR	423	6.788	8.770	35.408	1.00	10.93
ATOM	2599	CB	THR	423	5.663	7.746	35.699	1.00	11.82
ATOM	2600	OG1	THR	423	4.980	8.136	36.897	1.00	12.37
ATOM	2601	CG2	THR	423	6.228	6.335	35.876	1.00	12.10
ATOM	2602	C	THR	423	7.635	8.293	34.234	1.00	12.10
ATOM	2603	O	THR	423	7.219	8.376	33.078	1.00	10.45
ATOM	2604	N	PHE	424	8.825	7.792	34.541	1.00	8.77
ATOM	2605	CA	PHE	424	9.746	7.340	33.510	1.00	10.46
ATOM	2606	CB	PHE	424	10.432	8.562	32.883	1.00	12.06
ATOM	2607	CG	PHE	424	11.140	9.442	33.889	1.00	12.28
ATOM	2608	CD1	PHE	424	12.517	9.339	34.087	1.00	12.19
ATOM	2609	CD2	PHE	424	10.425	10.365	34.647	1.00	12.68
ATOM	2610	CE1	PHE	424	13.171	10.149	35.031	1.00	9.47
ATOM	2611	CE2	PHE	424	11.068	11.176	35.590	1.00	12.13
ATOM	2612	CZ	PHE	424	12.447	11.064	35.779	1.00	12.09
ATOM	2613	C	PHE	424	10.796	6.420	34.102	1.00	9.06
ATOM	2614	O	PHE	424	10.830	6.204	35.316	1.00	8.48
ATOM	2615	N	LEU	425	11.645	5.870	33.240	1.00	10.29
ATOM	2616	CA	LEU	425	12.726	5.004	33.697	1.00	12.71
ATOM	2617	CB	LEU	425	12.822	3.737	32.837	1.00	13.29
ATOM	2618	CG	LEU	425	13.418	2.518	33.552	1.00	15.65
ATOM	2619	CD1	LEU	425	12.484	2.088	34.676	1.00	13.51
ATOM	2620	CD2	LEU	425	13.618	1.374	32.576	1.00	14.52
ATOM	2621	C	LEU	425	14.019	5.811	33.578	1.00	12.49
ATOM	2622	O	LEU	425	14.213	6.557	32.610	1.00	13.19
ATOM	2623	N	PHE	426	14.887	5.688	34.575	1.00	13.60
ATOM	2624	CA	PHE	426	16.162	6.398	34.560	1.00	13.93
ATOM	2625	CB	PHE	426	16.133	7.620	35.484	1.00	15.88

ATOM	2626	CG	PHE	426	17.312	8.538	35.305	1.00	15.48
ATOM	2627	CD1	PHE	426	17.345	9.455	34.257	1.00	17.23
ATOM	2628	CD2	PHE	426	18.405	8.462	36.162	1.00	17.92
ATOM	2629	CE1	PHE	426	18.452	10.285	34.066	1.00	18.01
ATOM	2630	CE2	PHE	426	19.517	9.284	35.980	1.00	19.04
ATOM	2631	CZ	PHE	426	19.542	10.198	34.930	1.00	18.86
ATOM	2632	C	PHE	426	17.239	5.436	35.033	1.00	15.01
ATOM	2633	O	PHE	426	17.260	5.031	36.197	1.00	15.22
ATOM	2634	N	ARG	427	18.125	5.070	34.115	1.00	14.67
ATOM	2635	CA	ARG	427	19.208	4.150	34.405	1.00	15.02
ATOM	2636	CB	ARG	427	20.280	4.856	35.238	1.00	16.42
ATOM	2637	CG	ARG	427	20.754	6.148	34.584	1.00	17.28
ATOM	2638	CD	ARG	427	21.944	6.776	35.288	1.00	19.48
ATOM	2639	NE	ARG	427	23.162	5.984	35.142	1.00	21.16
ATOM	2640	CZ	ARG	427	24.357	6.384	35.564	1.00	20.91
ATOM	2641	NH1	ARG	427	24.484	7.563	36.153	1.00	20.35
ATOM	2642	NH2	ARG	427	25.422	5.609	35.402	1.00	20.64
ATOM	2643	C	ARG	427	18.691	2.900	35.113	1.00	14.73
ATOM	2644	O	ARG	427	19.237	2.474	36.128	1.00	14.34
ATOM	2645	N	GLY	428	17.619	2.332	34.565	1.00	14.44
ATOM	2646	CA	GLY	428	17.032	1.123	35.114	1.00	14.03
ATOM	2647	C	GLY	428	16.120	1.308	36.312	1.00	13.27
ATOM	2648	O	GLY	428	15.538	0.345	36.811	1.00	13.49
ATOM	2649	N	ARG	429	15.979	2.542	36.777	1.00	13.35
ATOM	2650	CA	ARG	429	15.136	2.800	37.934	1.00	12.19
ATOM	2651	CB	ARG	429	15.918	3.602	38.981	1.00	14.36
ATOM	2652	CG	ARG	429	15.052	4.235	40.056	1.00	14.95
ATOM	2653	CD	ARG	429	15.827	4.490	41.332	1.00	17.80
ATOM	2654	NE	ARG	429	17.121	5.145	41.134	1.00	17.56
ATOM	2655	CZ	ARG	429	18.097	5.115	42.039	1.00	17.08
ATOM	2656	NH1	ARG	429	17.912	4.468	43.181	1.00	16.54
ATOM	2657	NH2	ARG	429	19.258	5.713	41.806	1.00	17.47
ATOM	2658	C	ARG	429	13.838	3.514	37.590	1.00	10.01
ATOM	2659	O	ARG	429	13.817	4.432	36.770	1.00	9.48
ATOM	2660	N	ARG	430	12.750	3.072	38.210	1.00	9.28
ATOM	2661	CA	ARG	430	11.455	3.696	37.986	1.00	10.42
ATOM	2662	CB	ARG	430	10.319	2.778	38.442	1.00	11.00
ATOM	2663	CG	ARG	430	8.943	3.421	38.341	1.00	10.73
ATOM	2664	CD	ARG	430	8.665	3.909	36.920	1.00	9.69
ATOM	2665	NE	ARG	430	8.603	2.798	35.978	1.00	8.63
ATOM	2666	CZ	ARG	430	8.581	2.932	34.657	1.00	9.45
ATOM	2667	NH1	ARG	430	8.614	4.142	34.109	1.00	9.55
ATOM	2668	NH2	ARG	430	8.541	1.850	33.881	1.00	7.15
ATOM	2669	C	ARG	430	11.436	4.982	38.796	1.00	10.91
ATOM	2670	O	ARG	430	11.637	4.966	40.017	1.00	12.12
ATOM	2671	N	VAL	431	11.203	6.096	38.119	1.00	8.37
ATOM	2672	CA	VAL	431	11.189	7.382	38.796	1.00	9.63
ATOM	2673	CB	VAL	431	12.374	8.257	38.337	1.00	9.53
ATOM	2674	CG1	VAL	431	12.314	9.618	39.005	1.00	9.71
ATOM	2675	CG2	VAL	431	13.690	7.554	38.665	1.00	9.77
ATOM	2676	C	VAL	431	9.909	8.164	38.574	1.00	10.23
ATOM	2677	O	VAL	431	9.391	8.237	37.452	1.00	8.51
ATOM	2678	N	HIS	432	9.406	8.742	39.659	1.00	9.07
ATOM	2679	CA	HIS	432	8.209	9.569	39.622	1.00	9.74
ATOM	2680	CB	HIS	432	7.153	9.055	40.607	1.00	9.49
ATOM	2681	CG	HIS	432	6.709	7.652	40.346	1.00	11.50
ATOM	2682	CD2	HIS	432	6.923	6.508	41.039	1.00	10.25
ATOM	2683	ND1	HIS	432	5.964	7.299	39.243	1.00	11.07
ATOM	2684	CE1	HIS	432	5.740	5.997	39.265	1.00	10.85
ATOM	2685	NE2	HIS	432	6.310	5.493	40.344	1.00	11.44
ATOM	2686	C	HIS	432	8.591	10.992	40.030	1.00	9.91
ATOM	2687	O	HIS	432	8.702	11.289	41.221	1.00	12.14

ATOM	2688	N	LEU	433	8.826	11.863	39.055	1.00	10.10
ATOM	2689	CA	LEU	433	9.131	13.255	39.364	1.00	12.23
ATOM	2690	CB	LEU	433	9.632	14.002	38.118	1.00	11.65
ATOM	2691	CG	LEU	433	10.041	15.475	38.282	1.00	11.14
ATOM	2692	CD1	LEU	433	11.250	15.588	39.206	1.00	12.97
ATOM	2693	CD2	LEU	433	10.374	16.071	36.918	1.00	13.19
ATOM	2694	C	LEU	433	7.744	13.744	39.760	1.00	12.65
ATOM	2695	O	LEU	433	6.871	13.898	38.902	1.00	9.11
ATOM	2696	N	ALA	434	7.533	13.972	41.056	1.00	12.68
ATOM	2697	CA	ALA	434	6.216	14.385	41.530	1.00	12.21
ATOM	2698	CB	ALA	434	5.532	13.203	42.213	1.00	11.84
ATOM	2699	C	ALA	434	6.182	15.584	42.462	1.00	12.39
ATOM	2700	O	ALA	434	7.173	15.917	43.115	1.00	10.52
ATOM	2701	N	PRO	435	5.022	16.252	42.535	1.00	14.19
ATOM	2702	CD	PRO	435	3.824	16.070	41.689	1.00	12.75
ATOM	2703	CA	PRO	435	4.868	17.417	43.405	1.00	14.76
ATOM	2704	CB	PRO	435	3.741	18.186	42.734	1.00	15.35
ATOM	2705	CG	PRO	435	2.835	17.063	42.297	1.00	13.94
ATOM	2706	C	PRO	435	4.453	16.886	44.769	1.00	16.06
ATOM	2707	O	PRO	435	4.212	15.684	44.918	1.00	14.45
ATOM	2708	N	PRO	436	4.364	17.765	45.781	1.00	16.35
ATOM	2709	CD	PRO	436	4.714	19.195	45.812	1.00	16.70
ATOM	2710	CA	PRO	436	3.961	17.298	47.112	1.00	16.04
ATOM	2711	CB	PRO	436	3.988	18.572	47.950	1.00	16.31
ATOM	2712	CG	PRO	436	5.034	19.406	47.273	1.00	17.06
ATOM	2713	C	PRO	436	2.558	16.709	47.017	1.00	17.66
ATOM	2714	O	PRO	436	1.775	17.100	46.150	1.00	14.93
ATOM	2715	N	GLN	437	2.245	15.778	47.911	1.00	18.18
ATOM	2716	CA	GLN	437	0.945	15.115	47.927	1.00	20.53
ATOM	2717	CB	GLN	437	0.949	14.029	49.008	1.00	21.63
ATOM	2718	CG	GLN	437	-0.329	13.221	49.117	1.00	24.60
ATOM	2719	CD	GLN	437	-0.088	11.850	49.722	1.00	25.78
ATOM	2720	OE1	GLN	437	0.686	11.707	50.672	1.00	28.50
ATOM	2721	NE2	GLN	437	-0.753	10.836	49.178	1.00	22.40
ATOM	2722	C	GLN	437	-0.226	16.076	48.137	1.00	20.00
ATOM	2723	O	GLN	437	-1.392	15.680	48.062	1.00	20.52
ATOM	2724	N	THR	438	0.087	17.340	48.393	1.00	20.19
ATOM	2725	CA	THR	438	-0.942	18.347	48.600	1.00	19.99
ATOM	2726	CB	THR	438	-0.451	19.446	49.553	1.00	21.60
ATOM	2727	OG1	THR	438	0.805	19.949	49.088	1.00	20.45
ATOM	2728	CG2	THR	438	-0.287	18.893	50.966	1.00	22.05
ATOM	2729	C	THR	438	-1.362	18.986	47.277	1.00	20.72
ATOM	2730	O	THR	438	-2.185	19.904	47.256	1.00	18.84
ATOM	2731	N	TRP	439	-0.786	18.495	46.180	1.00	19.36
ATOM	2732	CA	TRP	439	-1.096	18.992	44.839	1.00	18.22
ATOM	2733	CB	TRP	439	-0.576	18.017	43.782	1.00	18.27
ATOM	2734	CG	TRP	439	-0.716	18.499	42.366	1.00	18.11
ATOM	2735	CD2	TRP	439	-1.790	18.211	41.459	1.00	18.54
ATOM	2736	CE2	TRP	439	-1.492	18.860	40.239	1.00	18.37
ATOM	2737	CE3	TRP	439	-2.972	17.465	41.559	1.00	18.86
ATOM	2738	CD1	TRP	439	0.159	19.292	41.680	1.00	19.09
ATOM	2739	NE1	TRP	439	-0.298	19.512	40.401	1.00	18.63
ATOM	2740	CZ2	TRP	439	-2.336	18.787	39.124	1.00	17.51
ATOM	2741	CZ3	TRP	439	-3.812	17.391	40.449	1.00	19.63
ATOM	2742	CH2	TRP	439	-3.487	18.051	39.246	1.00	18.63
ATOM	2743	C	TRP	439	-2.607	19.095	44.704	1.00	18.25
ATOM	2744	O	TRP	439	-3.332	18.194	45.121	1.00	19.31
ATOM	2745	N	ASP	440	-3.080	20.177	44.101	1.00	19.20
ATOM	2746	CA	ASP	440	-4.511	20.367	43.939	1.00	20.90
ATOM	2747	CB	ASP	440	-5.065	21.128	45.142	1.00	23.18
ATOM	2748	CG	ASP	440	-6.570	21.037	45.242	1.00	27.20
ATOM	2749	OD1	ASP	440	-7.154	21.762	46.074	1.00	29.35

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ATOM   2750  OD2 ASP   440      -7.168  20.232  44.494  1.00 29.14
ATOM   2751  C   ASP   440      -4.871  21.116  42.657  1.00 20.57
ATOM   2752  O   ASP   440      -5.585  22.119  42.699  1.00 21.05
ATOM   2753  N   GLY   441      -4.378  20.636  41.519  1.00 17.58
ATOM   2754  CA  GLY   441      -4.690  21.292  40.259  1.00 16.34
ATOM   2755  C   GLY   441      -3.512  21.997  39.614  1.00 16.68
ATOM   2756  O   GLY   441      -2.587  22.443  40.294  1.00 16.80
ATOM   2757  N   TYR   442      -3.550  22.113  38.290  1.00 15.98
ATOM   2758  CA  TYR   442      -2.471  22.753  37.555  1.00 14.71
ATOM   2759  CB  TYR   442      -2.471  22.276  36.102  1.00 13.29
ATOM   2760  CG  TYR   442      -2.140  20.814  35.947  1.00 11.43
ATOM   2761  CD1 TYR   442      -3.146  19.865  35.743  1.00 10.71
ATOM   2762  CE1 TYR   442      -2.836  18.508  35.604  1.00 11.58
ATOM   2763  CD2 TYR   442      -0.818  20.374  36.013  1.00 10.14
ATOM   2764  CE2 TYR   442      -0.500  19.032  35.879  1.00  9.35
ATOM   2765  CZ  TYR   442      -1.509  18.101  35.676  1.00 10.77
ATOM   2766  OH  TYR   442      -1.188  16.767  35.563  1.00  9.42
ATOM   2767  C   TYR   442      -2.519  24.276  37.585  1.00 15.48
ATOM   2768  O   TYR   442      -3.567  24.878  37.822  1.00 17.32
ATOM   2769  N   ASP   443      -1.369  24.889  37.333  1.00 14.75
ATOM   2770  CA  ASP   443      -1.250  26.344  37.316  1.00 15.10
ATOM   2771  CB  ASP   443      -0.265  26.800  38.393  1.00 15.62
ATOM   2772  CG  ASP   443      -0.296  28.297  38.612  1.00 16.83
ATOM   2773  OD1 ASP   443      -0.654  29.027  37.666  1.00 18.29
ATOM   2774  OD2 ASP   443       0.045  28.747  39.726  1.00 19.92
ATOM   2775  C   ASP   443      -0.736  26.762  35.945  1.00 14.68
ATOM   2776  O   ASP   443       0.447  26.607  35.644  1.00 17.52
ATOM   2777  N   PRO   444      -1.618  27.301  35.092  1.00 14.77
ATOM   2778  CD  PRO   444      -3.036  27.626  35.324  1.00 15.73
ATOM   2779  CA  PRO   444      -1.195  27.721  33.751  1.00 14.22
ATOM   2780  CB  PRO   444      -2.496  28.224  33.122  1.00 15.85
ATOM   2781  CG  PRO   444      -3.281  28.715  34.309  1.00 17.54
ATOM   2782  C   PRO   444      -0.074  28.757  33.731  1.00 13.23
ATOM   2783  O   PRO   444       0.558  28.970  32.698  1.00 14.12
ATOM   2784  N   SER   445       0.189  29.387  34.872  1.00 13.02
ATOM   2785  CA  SER   445       1.248  30.390  34.942  1.00 14.12
ATOM   2786  CB  SER   445       1.094  31.267  36.194  1.00 15.43
ATOM   2787  OG  SER   445       1.249  30.515  37.382  1.00 14.51
ATOM   2788  C   SER   445       2.617  29.718  34.935  1.00 15.13
ATOM   2789  O   SER   445       3.646  30.386  34.811  1.00 15.81
ATOM   2790  N   TRP   446       2.623  28.396  35.080  1.00 15.62
ATOM   2791  CA  TRP   446       3.867  27.628  35.045  1.00 16.04
ATOM   2792  CB  TRP   446       3.671  26.239  35.667  1.00 15.23
ATOM   2793  CG  TRP   446       3.790  26.180  37.179  1.00 15.78
ATOM   2794  CD2 TRP   446       4.492  25.187  37.948  1.00 14.80
ATOM   2795  CE2 TRP   446       4.303  25.502  39.313  1.00 15.90
ATOM   2796  CE3 TRP   446       5.261  24.064  37.613  1.00 13.03
ATOM   2797  CD1 TRP   446       3.221  27.032  38.088  1.00 18.10
ATOM   2798  NE1 TRP   446       3.526  26.630  39.371  1.00 17.03
ATOM   2799  CZ2 TRP   446       4.856  24.732  40.345  1.00 16.70
ATOM   2800  CZ3 TRP   446       5.811  23.298  38.638  1.00 14.05
ATOM   2801  CH2 TRP   446       5.604  23.637  39.989  1.00 14.48
ATOM   2802  C   TRP   446       4.175  27.486  33.561  1.00 15.56
ATOM   2803  O   TRP   446       3.544  26.692  32.870  1.00 15.44
ATOM   2804  N   THR   447       5.128  28.269  33.066  1.00 16.52
ATOM   2805  CA  THR   447       5.480  28.219  31.651  1.00 17.33
ATOM   2806  CB  THR   447       5.159  29.557  30.948  1.00 16.01
ATOM   2807  OG1 THR   447       5.880  30.621  31.583  1.00 19.51
ATOM   2808  CG2 THR   447       3.662  29.856  31.025  1.00 17.76
ATOM   2809  C   THR   447       6.951  27.895  31.427  1.00 17.48
ATOM   2810  O   THR   447       7.684  27.735  32.422  1.00 16.49
ATOM   2811  OT2 THR   447       7.350  27.808  30.248  1.00 20.48
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ATOM	2812	OH2	TIP	S	1	-2.614	14.475	15.320	1.00	6.09	S
ATOM	2813	OH2	TIP	S	2	-0.036	14.470	42.726	1.00	8.02	S
ATOM	2814	OH2	TIP	S	3	-5.358	21.667	30.895	1.00	12.21	S
ATOM	2815	OH2	TIP	S	4	-2.653	23.960	13.894	1.00	11.59	S
ATOM	2816	OH2	TIP	S	5	0.293	8.342	35.349	1.00	11.45	S
ATOM	2817	OH2	TIP	S	6	2.965	15.305	22.128	1.00	10.09	S
ATOM	2818	OH2	TIP	S	7	-13.868	20.810	25.262	1.00	10.29	S
ATOM	2819	OH2	TIP	S	8	9.042	7.228	29.895	1.00	8.92	S
ATOM	2820	OH2	TIP	S	9	-1.762	-4.348	15.634	1.00	4.51	S
ATOM	2821	OH2	TIP	S	10	1.296	9.499	31.865	1.00	11.62	S
ATOM	2822	OH2	TIP	S	11	1.765	13.754	2.497	1.00	6.99	S
ATOM	2823	OH2	TIP	S	12	-16.811	19.244	1.628	1.00	12.23	S
ATOM	2824	OH2	TIP	S	13	3.100	38.468	12.074	1.00	8.94	S
ATOM	2825	OH2	TIP	S	14	4.747	35.913	12.901	1.00	10.38	S
ATOM	2826	OH2	TIP	S	16	7.477	18.698	30.699	1.00	9.51	S
ATOM	2827	OH2	TIP	S	17	-1.635	-3.163	30.255	1.00	8.73	S
ATOM	2828	OH2	TIP	S	18	8.703	4.872	23.179	1.00	11.50	S
ATOM	2829	OH2	TIP	S	19	-1.885	11.655	14.762	1.00	8.17	S
ATOM	2830	OH2	TIP	S	20	-6.026	23.471	4.905	1.00	9.25	S
ATOM	2831	OH2	TIP	S	21	9.813	-5.306	24.495	1.00	14.00	S
ATOM	2832	OH2	TIP	S	22	7.572	25.441	29.067	1.00	14.85	S
ATOM	2833	OH2	TIP	S	23	-6.847	41.856	13.669	1.00	12.68	S
ATOM	2834	OH2	TIP	S	24	5.387	11.634	5.366	1.00	10.13	S
ATOM	2835	OH2	TIP	S	25	-3.336	18.278	28.003	1.00	11.28	S
ATOM	2836	OH2	TIP	S	26	3.576	28.559	8.666	1.00	16.37	S
ATOM	2837	OH2	TIP	S	27	-4.485	23.477	32.752	1.00	11.50	S
ATOM	2838	OH2	TIP	S	28	-0.469	15.386	17.048	1.00	8.13	S
ATOM	2839	OH2	TIP	S	29	8.632	14.162	-8.613	1.00	34.24	S
ATOM	2840	OH2	TIP	S	30	-5.058	-0.935	39.866	1.00	9.20	S
ATOM	2841	OH2	TIP	S	32	-2.306	20.625	28.936	1.00	14.92	S
ATOM	2842	OH2	TIP	S	33	6.559	-0.560	12.006	1.00	17.95	S
ATOM	2843	OH2	TIP	S	34	-14.668	9.195	27.132	1.00	10.60	S
ATOM	2844	OH2	TIP	S	35	10.046	9.125	17.048	1.00	18.33	S
ATOM	2845	OH2	TIP	S	36	7.551	17.754	-4.527	1.00	9.34	S
ATOM	2846	OH2	TIP	S	37	18.119	11.485	49.195	1.00	23.24	S
ATOM	2847	OH2	TIP	S	39	8.839	-0.876	35.357	1.00	19.31	S
ATOM	2848	OH2	TIP	S	40	-19.522	13.733	15.879	1.00	8.85	S
ATOM	2849	OH2	TIP	S	41	3.595	14.951	12.766	1.00	13.64	S
ATOM	2850	OH2	TIP	S	42	14.746	-1.569	29.631	1.00	17.35	S
ATOM	2851	OH2	TIP	S	43	2.428	16.587	4.597	1.00	8.45	S
ATOM	2852	OH2	TIP	S	44	2.533	4.050	9.665	1.00	9.99	S
ATOM	2853	OH2	TIP	S	46	2.392	26.208	30.638	1.00	18.05	S
ATOM	2854	OH2	TIP	S	47	3.005	4.365	-6.137	1.00	17.93	S
ATOM	2855	OH2	TIP	S	48	-9.349	26.333	11.553	1.00	15.39	S
ATOM	2856	OH2	TIP	S	49	16.813	3.154	31.969	1.00	15.56	S
ATOM	2857	OH2	TIP	S	50	-1.628	-7.357	12.842	1.00	15.27	S
ATOM	2858	OH2	TIP	S	51	-6.295	-4.666	35.782	1.00	11.85	S
ATOM	2859	OH2	TIP	S	52	3.718	17.317	-7.652	1.00	13.51	S
ATOM	2860	OH2	TIP	S	53	-4.530	1.420	38.605	1.00	16.40	S
ATOM	2861	OH2	TIP	S	55	5.219	-7.098	35.554	1.00	10.92	S
ATOM	2862	OH2	TIP	S	56	12.858	14.464	46.386	1.00	16.92	S
ATOM	2863	OH2	TIP	S	57	-6.993	13.007	38.760	1.00	21.66	S
ATOM	2864	OH2	TIP	S	59	1.946	-2.718	3.046	1.00	10.92	S
ATOM	2865	OH2	TIP	S	61	-13.046	10.832	22.809	1.00	15.93	S
ATOM	2866	OH2	TIP	S	62	-9.009	30.421	17.194	1.00	14.15	S
ATOM	2867	OH2	TIP	S	63	-5.368	14.834	28.617	1.00	15.13	S
ATOM	2868	OH2	TIP	S	64	15.902	7.116	22.062	1.00	15.93	S
ATOM	2869	OH2	TIP	S	65	-12.026	28.356	21.179	1.00	21.81	S
ATOM	2870	OH2	TIP	S	66	-21.274	19.841	17.262	1.00	17.46	S
ATOM	2871	OH2	TIP	S	67	2.502	9.579	35.754	1.00	11.78	S
ATOM	2872	OH2	TIP	S	71	17.599	6.826	25.546	1.00	24.21	S
ATOM	2873	OH2	TIP	S	73	-10.419	6.703	-3.028	1.00	18.73	S

ATOM	2874	OH2	TIP	S	76	-9.374	28.160	24.790	1.00	18.28	S
ATOM	2875	OH2	TIP	S	77	4.604	33.116	34.672	1.00	16.45	S
ATOM	2876	OH2	TIP	S	78	1.542	17.926	19.367	1.00	25.95	S
ATOM	2877	OH2	TIP	S	80	6.650	28.073	41.392	1.00	22.28	S
ATOM	2878	OH2	TIP	S	83	-19.029	6.784	19.748	1.00	23.80	S
ATOM	2879	OH2	TIP	S	84	3.507	18.590	5.884	1.00	17.30	S
ATOM	2880	OH2	TIP	S	85	-10.490	-4.096	26.776	1.00	22.45	S
ATOM	2881	OH2	TIP	S	86	-8.668	20.711	32.449	1.00	22.79	S
ATOM	2882	OH2	TIP	S	87	-12.608	13.926	-1.968	1.00	20.44	S
ATOM	2883	OH2	TIP	S	88	5.224	2.921	36.822	1.00	19.42	S
ATOM	2884	OH2	TIP	S	89	6.791	5.960	31.240	1.00	12.13	S
ATOM	2885	OH2	TIP	S	90	-16.107	17.938	6.363	1.00	12.89	S
ATOM	2886	OH2	TIP	S	91	6.958	9.725	30.511	1.00	15.40	S
ATOM	2887	OH2	TIP	S	93	3.503	35.440	17.011	1.00	15.08	S
ATOM	2888	OH2	TIP	S	94	3.974	9.960	33.442	1.00	12.24	S
ATOM	2889	OH2	TIP	S	95	2.755	10.650	26.918	1.00	14.89	S
ATOM	2890	OH2	TIP	S	96	11.034	25.614	42.827	1.00	18.93	S
ATOM	2891	OH2	TIP	S	97	0.170	2.551	35.237	1.00	13.32	S
ATOM	2892	OH2	TIP	S	98	-23.158	8.879	23.462	1.00	22.99	S
ATOM	2893	OH2	TIP	S	100	-3.421	-1.315	-5.473	1.00	28.16	S
ATOM	2894	OH2	TIP	S	102	6.509	15.318	13.449	1.00	15.11	S
ATOM	2895	OH2	TIP	S	105	-2.000	24.556	25.966	1.00	14.04	S
ATOM	2896	OH2	TIP	S	106	-12.623	17.738	-2.900	1.00	21.20	S
ATOM	2897	OH2	TIP	S	107	3.382	31.692	7.180	1.00	23.05	S
ATOM	2898	OH2	TIP	S	108	-7.135	8.901	-5.623	1.00	18.31	S
ATOM	2899	OH2	TIP	S	112	14.466	15.638	25.259	1.00	27.71	S
ATOM	2900	OH2	TIP	S	113	4.501	18.972	21.646	1.00	21.60	S
ATOM	2901	OH2	TIP	S	114	-18.595	22.604	23.180	1.00	26.96	S
ATOM	2902	OH2	TIP	S	115	2.021	42.650	13.021	1.00	18.30	S
ATOM	2903	OH2	TIP	S	117	9.096	-3.117	22.819	1.00	29.24	S
ATOM	2904	OH2	TIP	S	118	-9.458	11.657	37.718	1.00	31.53	S
ATOM	2905	OH2	TIP	S	119	0.906	-7.017	13.531	1.00	20.65	S
ATOM	2906	OH2	TIP	S	122	9.275	4.794	31.306	1.00	20.24	S
ATOM	2907	OH2	TIP	S	123	15.065	18.264	29.279	1.00	20.60	S
ATOM	2908	OH2	TIP	S	124	-12.335	22.939	7.049	1.00	27.49	S
ATOM	2909	OH2	TIP	S	125	-5.724	-5.533	5.290	1.00	27.47	S
ATOM	2910	OH2	TIP	S	126	12.084	3.404	16.865	1.00	23.96	S
ATOM	2911	OH2	TIP	S	128	-8.595	-11.278	22.093	1.00	26.86	S
ATOM	2912	OH2	TIP	S	129	5.131	1.124	-1.218	1.00	21.59	S
ATOM	2913	OH2	TIP	S	132	-7.436	27.713	10.184	1.00	18.40	S
ATOM	2914	OH2	TIP	S	133	-8.171	12.632	34.731	1.00	29.10	S
ATOM	2915	OH2	TIP	S	135	-4.836	24.044	1.758	1.00	14.59	S
ATOM	2916	OH2	TIP	S	137	-7.765	35.235	11.118	1.00	17.63	S
ATOM	2917	OH2	TIP	S	141	2.152	-1.255	0.907	1.00	23.02	S
ATOM	2918	OH2	TIP	S	145	18.041	6.066	31.696	1.00	21.56	S
ATOM	2919	OH2	TIP	S	146	10.748	9.252	51.746	1.00	20.23	S
ATOM	2920	OH2	TIP	S	149	6.417	14.065	46.284	1.00	24.04	S
ATOM	2921	OH2	TIP	S	150	3.909	14.492	49.629	1.00	23.43	S
ATOM	2922	OH2	TIP	S	151	6.877	17.130	10.801	1.00	24.56	S
ATOM	2923	OH2	TIP	S	152	-14.741	11.032	25.129	1.00	16.30	S
ATOM	2924	OH2	TIP	S	155	3.111	34.806	35.976	1.00	13.40	S
ATOM	2925	OH2	TIP	S	156	4.969	20.254	4.177	1.00	22.40	S
ATOM	2926	OH2	TIP	S	157	4.016	0.044	27.035	1.00	16.07	S
ATOM	2927	OH2	TIP	S	158	-9.363	34.561	16.436	1.00	25.93	S
ATOM	2928	OH2	TIP	S	160	19.264	7.927	30.593	1.00	16.82	S
ATOM	2929	OH2	TIP	S	161	10.873	-2.091	21.405	1.00	28.45	S
ATOM	2930	OH2	TIP	S	162	7.187	32.913	35.096	1.00	30.28	S
ATOM	2931	OH2	TIP	S	163	9.841	19.050	11.607	1.00	25.04	S
ATOM	2932	OH2	TIP	S	164	7.677	1.935	3.185	1.00	32.57	S
ATOM	2933	OH2	TIP	S	165	-15.785	12.920	28.289	1.00	21.09	S
ATOM	2934	OH2	TIP	S	166	4.494	22.439	2.979	1.00	22.71	S
ATOM	2935	OH2	TIP	S	167	1.974	19.423	-7.665	1.00	25.54	S

ATOM	2936	OH2	TIP	S	168	-17.521	22.873	25.644	1.00	30.27	S
ATOM	2937	OH2	TIP	S	169	-20.674	9.651	14.274	1.00	18.18	S
ATOM	2938	OH2	TIP	S	170	-6.859	-2.770	39.309	1.00	16.58	S
ATOM	2939	OH2	TIP	S	171	22.405	2.426	50.167	1.00	33.80	S
ATOM	2940	OH2	TIP	S	176	18.678	16.924	23.159	1.00	32.68	S
ATOM	2941	OH2	TIP	S	178	3.668	2.300	-7.962	1.00	25.82	S
ATOM	2942	OH2	TIP	S	179	14.990	16.379	45.492	1.00	36.75	S
ATOM	2943	OH2	TIP	S	180	5.773	2.145	46.020	1.00	22.60	S
ATOM	2944	OH2	TIP	S	182	18.955	6.194	39.240	1.00	18.76	S
ATOM	2945	OH2	TIP	S	183	3.010	-10.168	29.047	1.00	21.32	S
ATOM	2946	OH2	TIP	S	184	20.011	4.284	31.088	1.00	26.65	S
ATOM	2947	OH2	TIP	S	185	-12.403	27.389	24.081	1.00	30.69	S
ATOM	2948	OH2	TIP	S	186	-12.441	21.757	-4.228	1.00	21.82	S
ATOM	2949	OH2	TIP	S	187	-13.219	10.479	-2.886	1.00	34.62	S
ATOM	2950	OH2	TIP	S	188	1.558	12.971	27.484	1.00	24.57	S
ATOM	2951	OH2	TIP	S	189	-19.186	1.476	13.722	1.00	27.29	S
ATOM	2952	OH2	TIP	S	190	13.683	6.943	10.471	1.00	33.74	S
ATOM	2953	OH2	TIP	S	191	11.723	-2.258	23.786	1.00	42.12	S
ATOM	2954	OH2	TIP	S	192	6.559	-9.147	18.487	1.00	27.37	S
ATOM	2955	OH2	TIP	S	194	-12.453	0.925	-0.905	1.00	34.57	S
ATOM	2956	OH2	TIP	S	195	6.896	14.419	22.729	1.00	24.07	S
ATOM	2957	OH2	TIP	S	196	-17.331	3.605	34.093	1.00	35.10	S
ATOM	2958	OH2	TIP	S	197	15.286	25.898	37.100	1.00	33.19	S
ATOM	2959	OH2	TIP	S	198	-4.010	12.845	-9.138	1.00	34.17	S
ATOM	2960	OH2	TIP	S	199	-7.321	32.975	16.990	1.00	26.97	S
ATOM	2961	OH2	TIP	S	201	-6.764	-7.564	6.737	1.00	35.93	S
ATOM	2962	OH2	TIP	S	202	-7.549	17.049	44.135	1.00	28.48	S
ATOM	2963	OH2	TIP	S	204	-19.943	5.202	6.054	1.00	28.41	S
ATOM	2964	OH2	TIP	S	205	-11.193	27.279	-3.127	1.00	39.41	S
ATOM	2965	OH2	TIP	S	206	-1.108	6.732	-9.043	1.00	24.53	S
ATOM	2966	OH2	TIP	S	207	17.585	5.364	20.588	1.00	29.42	S
ATOM	2967	OH2	TIP	S	208	-3.225	-1.757	-2.933	1.00	27.98	S
ATOM	2968	OH2	TIP	S	211	-5.067	15.672	-3.972	1.00	23.60	S
ATOM	2969	OH2	TIP	S	212	12.040	1.253	45.854	1.00	25.81	S
ATOM	2970	OH2	TIP	S	213	5.253	21.577	42.993	1.00	25.22	S
ATOM	2971	OH2	TIP	S	214	-10.202	-4.405	29.925	1.00	29.96	S
ATOM	2972	OH2	TIP	S	215	-2.463	14.056	44.322	1.00	26.90	S
ATOM	2973	OH2	TIP	S	216	-19.468	19.594	3.031	1.00	27.12	S
ATOM	2974	OH2	TIP	S	217	20.356	6.576	24.151	1.00	32.90	S
ATOM	2975	OH2	TIP	S	218	-9.237	-10.666	35.339	1.00	22.89	S
ATOM	2976	OH2	TIP	S	220	-18.889	17.888	6.460	1.00	30.59	S
ATOM	2977	OH2	TIP	S	222	-8.146	-1.501	-6.675	1.00	43.27	S
ATOM	2978	OH2	TIP	S	223	4.190	-9.371	24.429	1.00	21.84	S
ATOM	2979	OH2	TIP	S	224	-5.519	24.812	34.841	1.00	31.56	S
ATOM	2980	OH2	TIP	S	226	11.269	8.066	5.149	1.00	30.92	S
ATOM	2981	OH2	TIP	S	227	8.741	16.773	13.800	1.00	31.52	S
ATOM	2982	OH2	TIP	S	228	-7.860	31.822	23.573	1.00	32.45	S
ATOM	2983	OH2	TIP	S	230	-4.838	7.069	46.879	1.00	32.19	S
ATOM	2984	OH2	TIP	S	231	10.253	1.539	7.902	1.00	36.38	S
ATOM	2985	OH2	TIP	S	232	-1.486	22.411	42.677	1.00	20.68	S
ATOM	2986	OH2	TIP	S	233	-8.823	33.642	4.827	1.00	26.06	S
ATOM	2987	OH2	TIP	S	234	-20.801	15.966	16.129	1.00	28.25	S
ATOM	2988	OH2	TIP	S	236	0.861	21.703	46.935	1.00	30.57	S
ATOM	2989	OH2	TIP	S	237	-17.163	-0.156	27.372	1.00	23.51	S
ATOM	2990	OH2	TIP	S	238	-13.191	-1.432	5.324	1.00	39.15	S
ATOM	2991	OH2	TIP	S	239	6.272	-7.471	31.762	1.00	23.96	S
ATOM	2992	OH2	TIP	S	241	-2.301	8.523	-10.613	1.00	29.15	S
ATOM	2993	OH2	TIP	S	242	1.722	13.681	52.922	1.00	36.22	S
ATOM	2994	OH2	TIP	S	244	8.310	-0.211	39.413	1.00	27.76	S
ATOM	2995	OH2	TIP	S	246	-15.776	-1.194	7.321	1.00	26.89	S
ATOM	2996	OH2	TIP	S	249	-6.558	18.990	-1.378	1.00	24.02	S
ATOM	2997	OH2	TIP	S	250	-17.741	15.046	24.611	1.00	26.61	S

ATOM	2998	OH2	TIP	S	253	-5.486	-4.379	2.498	1.00	25.72	S
ATOM	2999	OH2	TIP	S	254	-5.892	4.867	-3.600	1.00	30.28	S
ATOM	3000	OH2	TIP	S	259	7.639	15.112	-4.183	1.00	19.48	S
ATOM	3001	OH2	TIP	S	260	17.966	8.018	16.377	1.00	50.14	S
ATOM	3002	OH2	TIP	S	262	6.927	6.927	51.120	1.00	36.10	S
ATOM	3003	OH2	TIP	S	263	12.270	12.800	27.411	1.00	38.90	S
ATOM	3004	OH2	TIP	S	264	-9.913	4.116	-3.359	1.00	35.97	S
ATOM	3005	OH2	TIP	S	266	-19.276	18.340	15.646	1.00	23.56	S
ATOM	3006	OH2	TIP	S	267	-16.663	12.896	25.800	1.00	20.01	S
ATOM	3007	OH2	TIP	S	270	-2.312	29.497	25.547	1.00	13.85	S
ATOM	3008	OH2	TIP	S	271	18.495	14.333	23.517	1.00	24.52	S
ATOM	3009	OH2	TIP	S	273	19.487	2.148	39.357	1.00	21.73	S
ATOM	3010	OH2	TIP	S	275	5.526	-11.397	20.474	1.00	40.91	S
ATOM	3011	OH2	TIP	S	276	7.711	29.938	34.474	1.00	22.25	S
ATOM	3012	OH2	TIP	S	278	-10.024	29.043	4.853	1.00	20.31	S
ATOM	3013	OH2	TIP	S	279	-9.570	35.739	3.011	1.00	24.60	S
ATOM	3014	OH2	TIP	S	280	-8.330	-5.504	27.111	1.00	27.85	S
ATOM	3015	OH2	TIP	S	281	-12.008	-2.272	29.037	1.00	28.01	S
ATOM	3016	OH2	TIP	S	282	-18.223	17.511	0.409	1.00	44.50	S
ATOM	3017	OH2	TIP	S	283	9.967	32.965	36.408	1.00	32.45	S
ATOM	3018	OH2	TIP	S	284	-20.025	20.841	25.208	1.00	32.55	S
ATOM	3019	OH2	TIP	S	285	-3.135	-3.705	1.137	1.00	29.29	S
ATOM	3020	OH2	TIP	S	286	-15.605	-0.858	36.573	1.00	31.30	S
ATOM	3021	OH2	TIP	S	287	22.736	8.293	50.227	1.00	42.33	S
ATOM	3022	OH2	TIP	S	288	17.524	0.865	40.770	1.00	28.19	S
ATOM	3023	OH2	TIP	S	289	7.381	0.344	-0.365	1.00	38.81	S
ATOM	3024	OH2	TIP	S	290	-9.434	31.287	3.731	1.00	29.14	S
ATOM	3025	OH2	TIP	S	292	14.395	0.506	26.802	1.00	31.68	S
ATOM	3026	OH2	TIP	S	293	-18.885	7.379	26.307	1.00	34.11	S
ATOM	3027	OH2	TIP	S	294	1.506	21.499	44.520	1.00	27.32	S
ATOM	3028	OH2	TIP	S	295	-15.165	28.115	15.669	1.00	24.48	S
ATOM	3029	OH2	TIP	S	296	-3.176	23.510	44.563	1.00	34.08	S
ATOM	3030	OH2	TIP	S	297	28.692	6.135	44.148	1.00	34.24	S
ATOM	3031	OH2	TIP	S	298	-21.550	6.040	14.130	1.00	40.59	S
ATOM	3032	OH2	TIP	S	299	-16.657	27.596	24.184	1.00	40.98	S
ATOM	3033	OH2	TIP	S	300	2.591	21.757	42.148	1.00	27.88	S
ATOM	3034	OH2	TIP	S	301	24.297	5.640	49.289	1.00	50.83	S
ATOM	3035	OH2	TIP	S	302	17.500	18.253	10.340	1.00	35.00	S
ATOM	3036	OH2	TIP	S	303	21.687	0.862	37.246	1.00	32.98	S
ATOM	3037	OH2	TIP	S	304	-17.710	13.870	29.687	1.00	33.06	S
ATOM	3038	OH2	TIP	S	305	-9.948	28.208	7.254	1.00	39.84	S
ATOM	3039	OH2	TIP	S	306	14.234	-1.991	39.400	1.00	39.52	S
ATOM	3040	OH2	TIP	S	307	-6.703	29.552	17.319	1.00	26.55	S
ATOM	3041	OH2	TIP	S	308	3.310	6.855	-7.683	1.00	29.35	S
ATOM	3042	OH2	TIP	S	309	13.321	25.980	44.243	1.00	31.85	S
ATOM	3043	C1	MAN	X	501	3.440	22.064	17.321	1.00	50.88	X
ATOM	3044	C2	MAN	X	501	2.691	21.140	18.265	1.00	48.50	X
ATOM	3045	O2	MAN	X	501	2.239	20.000	17.561	1.00	50.47	X
ATOM	3046	C3	MAN	X	501	3.626	20.714	19.388	1.00	43.43	X
ATOM	3047	O3	MAN	X	501	2.960	19.787	20.229	1.00	41.15	X
ATOM	3048	C4	MAN	X	501	4.907	20.079	18.827	1.00	41.19	X
ATOM	3049	O4	MAN	X	501	5.832	19.915	19.888	1.00	43.86	X
ATOM	3050	C5	MAN	X	501	5.551	20.961	17.744	1.00	42.11	X
ATOM	3051	O5	MAN	X	501	4.564	21.375	16.771	1.00	47.10	X
ATOM	3052	C6	MAN	X	501	6.647	20.230	16.986	1.00	40.18	X
ATOM	3053	O6	MAN	X	501	7.161	21.023	15.924	1.00	38.11	X
ATOM	3054	C1	MAN	V	502	-0.753	27.426	26.438	1.00	71.88	V
ATOM	3055	C2	MAN	V	502	-0.025	27.235	27.787	1.00	65.50	V
ATOM	3056	O2	MAN	V	502	1.353	27.536	27.640	1.00	64.12	V
ATOM	3057	C3	MAN	V	502	-0.628	28.096	28.909	1.00	61.97	V
ATOM	3058	O3	MAN	V	502	0.329	29.029	29.391	1.00	56.59	V
ATOM	3059	C4	MAN	V	502	-1.875	28.833	28.423	1.00	63.11	V

ATOM	3060	O4	MAN	V	502	-2.537	29.420	29.534	1.00	59.04	V
ATOM	3061	C5	MAN	V	502	-2.811	27.844	27.727	1.00	68.52	V
ATOM	3062	O5	MAN	V	502	-2.163	27.198	26.591	1.00	70.43	V
ATOM	3063	C6	MAN	V	502	-4.093	28.476	27.218	1.00	70.50	V
ATOM	3064	O6	MAN	V	502	-4.561	29.495	28.090	1.00	78.59	V
ATOM	3065	C1	MAN	Y	503	3.095	26.825	17.689	1.00	84.76	Y
ATOM	3066	C2	MAN	Y	503	3.900	25.547	17.635	1.00	88.64	Y
ATOM	3067	O2	MAN	Y	503	4.915	25.580	18.629	1.00	91.25	Y
ATOM	3068	C3	MAN	Y	503	2.989	24.344	17.859	1.00	88.68	Y
ATOM	3069	O3	MAN	Y	503	3.822	23.196	18.036	1.00	88.70	Y
ATOM	3070	C4	MAN	Y	503	2.068	24.517	19.091	1.00	87.64	Y
ATOM	3071	O4	MAN	Y	503	1.080	23.496	19.091	1.00	90.14	Y
ATOM	3072	C5	MAN	Y	503	1.387	25.891	19.034	1.00	85.70	Y
ATOM	3073	O5	MAN	Y	503	2.393	26.905	18.938	1.00	84.76	Y
ATOM	3074	C6	MAN	Y	503	0.426	26.272	20.168	1.00	85.98	Y
ATOM	3075	O6	MAN	Y	503	1.135	26.764	21.334	1.00	85.02	Y
ATOM	3076	C1	MAN	U	504	-3.865	28.519	19.532	1.00	71.88	U
ATOM	3077	C2	MAN	U	504	-3.642	29.725	18.613	1.00	65.50	U
ATOM	3078	O2	MAN	U	504	-4.290	29.513	17.367	1.00	64.12	U
ATOM	3079	C3	MAN	U	504	-4.182	30.997	19.275	1.00	61.97	U
ATOM	3080	O3	MAN	U	504	-4.103	32.078	18.357	1.00	56.59	U
ATOM	3081	C4	MAN	U	504	-5.633	30.818	19.736	1.00	63.11	U
ATOM	3082	O4	MAN	U	504	-6.001	31.909	20.562	1.00	59.04	U
ATOM	3083	C5	MAN	U	504	-5.830	29.520	20.528	1.00	68.52	U
ATOM	3084	O5	MAN	U	504	-5.259	28.393	19.822	1.00	70.43	U
ATOM	3085	C6	MAN	U	504	-7.300	29.221	20.740	1.00	70.50	U
ATOM	3086	O6	MAN	U	504	-8.122	30.136	20.030	1.00	78.59	U
ATOM	3087	C1	MAN	W	512	0.538	27.870	21.981	1.00	88.26	W
ATOM	3088	C2	MAN	W	512	0.685	27.753	23.514	1.00	82.56	W
ATOM	3089	O2	MAN	W	512	0.467	29.026	24.106	1.00	83.59	W
ATOM	3090	C3	MAN	W	512	-0.336	26.747	24.065	1.00	77.23	W
ATOM	3091	O3	MAN	W	512	-0.180	26.548	25.498	1.00	67.76	W
ATOM	3092	C4	MAN	W	512	-1.750	27.189	23.677	1.00	78.70	W
ATOM	3093	O4	MAN	W	512	-2.710	26.281	24.199	1.00	76.59	W
ATOM	3094	C5	MAN	W	512	-1.804	27.187	22.147	1.00	83.18	W
ATOM	3095	O5	MAN	W	512	-0.830	28.119	21.609	1.00	85.83	W
ATOM	3096	C6	MAN	W	512	-3.177	27.541	21.582	1.00	89.02	W
ATOM	3097	O6	MAN	W	512	-3.083	28.668	20.689	1.00	98.12	W
ATOM	3098	C1	NAG	Z	515	4.015	31.757	18.793	1.00	60.43	Z
ATOM	3099	C2	NAG	Z	515	5.207	30.952	19.337	1.00	62.23	Z
ATOM	3100	N2	NAG	Z	515	6.457	31.649	19.134	1.00	56.94	Z
ATOM	3101	C7	NAG	Z	515	7.585	31.172	19.655	1.00	52.95	Z
ATOM	3102	O7	NAG	Z	515	7.888	31.315	20.838	1.00	54.95	Z
ATOM	3103	C8	NAG	Z	515	8.524	30.428	18.722	1.00	51.24	Z
ATOM	3104	C3	NAG	Z	515	5.257	29.617	18.603	1.00	68.39	Z
ATOM	3105	O3	NAG	Z	515	6.227	28.772	19.203	1.00	69.66	Z
ATOM	3106	C4	NAG	Z	515	3.905	28.901	18.601	1.00	71.84	Z
ATOM	3107	O4	NAG	Z	515	3.945	27.907	17.569	1.00	81.22	Z
ATOM	3108	C5	NAG	Z	515	2.720	29.850	18.325	1.00	69.64	Z
ATOM	3109	O5	NAG	Z	515	2.843	31.032	19.104	1.00	65.24	Z
ATOM	3110	C6	NAG	Z	515	1.362	29.264	18.676	1.00	71.31	Z
ATOM	3111	O6	NAG	Z	515	0.751	29.957	19.757	1.00	73.67	Z
ATOM	3112	C1	NAG	A	516	0.539	35.554	19.965	1.00	52.78	A
ATOM	3113	O1	NAG	A	516	0.706	35.742	21.329	1.00	17.20	A
ATOM	3114	C2	NAG	A	516	0.205	34.076	19.676	1.00	55.38	A
ATOM	3115	N2	NAG	A	516	-0.512	33.525	20.813	1.00	53.49	A
ATOM	3116	C7	NAG	A	516	-0.929	32.262	20.797	1.00	54.05	A
ATOM	3117	O7	NAG	A	516	-1.692	31.829	19.937	1.00	55.49	A
ATOM	3118	C8	NAG	A	516	-0.424	31.331	21.892	1.00	53.24	A
ATOM	3119	C3	NAG	A	516	1.407	33.145	19.366	1.00	59.86	A
ATOM	3120	O3	NAG	A	516	1.037	32.314	18.278	1.00	63.08	A
ATOM	3121	C4	NAG	A	516	2.761	33.832	19.024	1.00	63.50	A

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ATOM   3122  O4  NAG A 516       3.893  32.997  19.408  1.00 72.74      A
ATOM   3123  C5  NAG A 516       2.825  35.151  19.755  1.00 61.66      A
ATOM   3124  O5  NAG A 516       1.736  35.957  19.319  1.00 57.10      A
ATOM   3125  C6  NAG A 516       4.080  35.947  19.585  1.00 62.55      A
ATOM   3126  O6  NAG A 516       3.836  37.321  19.825  1.00 63.27      A
ATOM   3127  C1' UD1   449       2.919  19.664  14.585  1.00 30.17
ATOM   3128  C2' UD1   449       2.470  18.369  15.271  1.00 31.67
ATOM   3129  C3' UD1   449       1.153  17.920  14.628  1.00 29.55
ATOM   3130  C4' UD1   449       0.031  18.972  14.749  1.00 27.43
ATOM   3131  C5' UD1   449       0.560  20.417  14.389  1.00 26.95
ATOM   3132  C6' UD1   449      -0.328  21.493  15.010  1.00 25.22
ATOM   3133  C7' UD1   449       4.047  16.896  16.375  1.00 36.58
ATOM   3134  C8' UD1   449       5.105  15.871  16.235  1.00 36.04
ATOM   3135  N2' UD1   449       3.481  17.288  15.241  1.00 34.73
ATOM   3136  O1' UD1   449       3.035  19.430  13.167  1.00 29.11
ATOM   3137  O3' UD1   449       0.789  16.688  15.267  1.00 32.87
ATOM   3138  O4' UD1   449      -0.978  18.658  13.783  1.00 22.83
ATOM   3139  O5' UD1   449       1.940  20.677  14.818  1.00 30.11
ATOM   3140  O6' UD1   449      -0.163  22.698  14.267  1.00 22.21
ATOM   3141  O7' UD1   449       3.670  17.236  17.507  1.00 34.89
ATOM   3142  N1  UD1   449      -0.675  19.435   6.886  1.00 13.55
ATOM   3143  C2  UD1   449      -1.869  19.855   6.304  1.00 13.16
ATOM   3144  N3  UD1   449      -1.841  20.980   5.574  1.00 12.14
ATOM   3145  C4  UD1   449      -0.776  21.768   5.366  1.00 13.78
ATOM   3146  C5  UD1   449       0.523  21.374   5.953  1.00 15.04
ATOM   3147  C6  UD1   449       0.574  20.242   6.697  1.00 13.86
ATOM   3148  O2  UD1   449      -2.955  19.293   6.419  1.00 14.23
ATOM   3149  O4  UD1   449      -0.859  22.730   4.614  1.00 12.86
ATOM   3150  C1* UD1   449      -0.651  18.192   7.687  1.00 14.93
ATOM   3151  C2* UD1   449       0.496  17.207   7.363  1.00 13.22
ATOM   3152  O2* UD1   449       0.143  16.450   6.194  1.00 14.37
ATOM   3153  C3* UD1   449       0.615  16.401   8.681  1.00 14.29
ATOM   3154  C4* UD1   449       0.139  17.427   9.745  1.00 14.97
ATOM   3155  O4* UD1   449      -0.534  18.483   9.060  1.00 13.43
ATOM   3156  O3* UD1   449      -0.330  15.327   8.642  1.00 16.70
ATOM   3157  C5* UD1   449       1.320  18.119  10.503  1.00 15.80
ATOM   3158  O5* UD1   449       2.300  18.744   9.647  1.00 15.45
ATOM   3159  PA  UD1   449       3.840  18.566   9.826  1.00 18.59
ATOM   3160  O1A UD1   449       4.414  18.996   8.518  1.00 14.88
ATOM   3161  O2A UD1   449       4.146  17.168  10.092  1.00 16.57
ATOM   3162  O3A UD1   449       4.257  19.452  10.954  1.00 19.35
ATOM   3163  PB  UD1   449       4.449  19.218  12.489  1.00 25.38
ATOM   3164  O1B UD1   449       5.459  20.138  13.059  1.00 28.03
ATOM   3165  O2B UD1   449       4.753  17.787  12.765  1.00 21.55
ATOM   3166 MN+2 MN2   448       5.258  16.175  11.593  1.00 13.36
ATOM   3167  N   ILE   113      -3.786  11.902   7.815  0.50  7.78      AC2
ATOM   3168  CA  ILE   113      -3.713  13.286   7.360  0.50  7.25      AC2
ATOM   3169  CB  ILE   113      -3.651  14.267   8.555  0.50  6.73      AC2
ATOM   3170  CG2 ILE   113      -3.633  15.708   8.051  0.50  6.66      AC2
ATOM   3171  CG1 ILE   113      -4.858  14.050   9.473  0.50  4.62      AC2
ATOM   3172  CD1 ILE   113      -6.196  14.256   8.790  0.50  2.31      AC2
ATOM   3173  C   ILE   113      -2.458  13.445   6.508  0.50  8.03      AC2
ATOM   3174  O   ILE   113      -1.350  13.164   6.965  0.50  7.50      AC2
END
```

Table 5 Intermolecular contacts of GnT-1-UDP-GlcNAc Complex and GnT-1-$Man_5GlcNAc_2$ Complex

No. of Atomic Interaction	Nucleotide Sugar Donor or Acceptor Atomic Contact	Enzyme Atomic Contact	Distance Between Atomic Contacts	Atomic Interaction Property
1	Uracil O2	His-190 ND1	2.7	HB
2	Uracil N3	Asp 144	2.8	HB
3	Uracil Ring	Cys 115 - Cys 145	3.7	VW
4		Ile 187	3.8	VW
5	Uracil C5	Val 321	3.6	VW
6	Ribose O3'(H)	Asp 212	2.9	HB
7	O2'(H)	Asp 212	3.2 direct, and via water: 2.9 to water, & 3.0 to Asp212	HB HB HB
8	α Phosphate	Arg 117 NH	2.8	SB
9		Val 321	2.7	HB
10	β-phosphate	Ser 322	2.5	HB
	Loop Structure			
11	α-phosphate	Val 321	2.7	HB
12		Asp 116	via 2.8 water, 2.8 to second water, 2.7 to Asp	HB, HB HB
13	β-phosphate	Ser 322	2.5	HB
14	GlcNAc O3	Glu 211	2.7	HB
15	O6	Phe 289,	via 2.7 to water , 2.8	HB, HB
16		Trp 290	3.2	HB
17		Tyr 184	2.9	HB
18	O4	Glu 211	2.6	HB
19		Trp 290	2.8	HB
20	CH_3	Leu 269	3.4	VW
21		Leu 331	3.3	VW
	α-1,3, mannose			
22	O2	Asp 291 OD1	2.4	HB
23	O3	Asp291	3.1	HB
24		Arg 295	2.9	HB
25	O4	Arg 415	via 2.6 water 2.5 to Arg	HB
26	O6	Ser 322		HB
27	C6	Phe 326	2.6 3.6	VW

HB: hydrogen bond interaction
VW Nad der Waals
SB: salt bridge

Table 6 Crystallographic data and refinement statistics.

	Derivative (MeHgCl)			
	Edge	Peak	Native	Complex with UDP-GlcNAc and Mn^{2+}
Crystal parameters:				
Space group	$P2_12_12_1$		$P2_12_12_1$	$P2_12_12_1$
α (Å)	40.4		40.5	40.5
β (Å)	82.4		82.4	82.2
γ (Å)	102.5		102.5	102.0
Diffraction statistics:				
Wavelength (Å)	1.0093	1.0075	0.9914	1.0713
Resolution Range (Å)	31.72 – 1.4	31.72 – 1.4	38.24 – 1.5	34.25 – 1.8
Measured reflections (n)	348028	325287	401605	64537
Unique relections (n)	102627	102233	99934	42919
Completeness (%)	78.7	78.4	94.2	70.3
R_{sym}*	0.047	0.053	0.065	0.092
Sites (n)	1	1	-	-
Phasing Power†:				
Dispersive	-	1.64	-	-
Anomalous	2.26	2.65	-	-
Figure of Merit, before Solvent flattening	0.581	-	-	-
Refinement statistics:				
R_{cryst}	0.167	-	0.166	0.185
R_{free}	0.189	-	0.194	0.229
Total atoms (n)	3204	-	3167	3138
Protein	2710	-	2710	2811
Substrate	0	-	0	40
Water	492	-	457	275
Rmsd‡ bond length (Å)	0.011	-	0.013	0.010
Rmsd bond angle (°)	1.5	-	1.6	1.5
Mean B value (Å²)	14.2	-	14.4	16.2
Protein	12.3	-	12.3	16.0
Domain 1 (106-317)	11.5	-	11.3	14.2
Loop (318-330)	-	-	-	28.3
Linker (331-353)	12.1	-	12.1	15.4
Domain 2 (354-447)	14.1	-	14.6	18.7
Substrates	-	-	-	23.0
Water	26.6	-	27.9	25.9

* $R_{sym} = \quad |I - \langle I \rangle| / \quad I$, where I is the observed intensity and $\langle I \rangle$ is the average intensity obtained from multiple observations of symmetry-related reflections. † Phasing power, root mean square (rms) F_H/rms ε, where ε is lack of closure and F_H is the calculated heavy atom structure factor. ‡ Rmsd, root mean squared deviation

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Table 7

The UDP-GlcNAc binding site. Listed here are the distances between the UDP-GlcNAc, the Mn^{2+}, bound waters, and the protein atoms involved in their binding.

Interacting Atoms		Distance (Å)	Interacting Atoms		Distance (Å)
Uracil N3	D144 OD2	2.8	GlcNAc O6	H_2O 4	2.7
Uracil O2	H190 ND1	2.7	Mn^{2+}	D213 OD2	2.1
Ribose O2'	D212 OD1	3.2	Mn^{2+}	H_2O 38	2.4
Ribose O2'	H_2O 40	2.9	Mn^{2+}	H_2O 87	2.4
Ribose O3'	D212 OD1	2.9	Mn^{2+}	H_2O 116	2.1
α-Phosphate O1A	V321 N	2.7	H_2O 4	Y184 O	2.9
α-Phosphate O1A	H2O 72	2.8	H_2O 4	F289 N	2.8
α-Phosphate O2A	R117 NH2	2.8	H_2O 4	W290 N	3.2
α-Phosphate O2A	Mn^{2+}	2.1	H_2O 27	L269 N	3.0
β-Phosphate O1B	S322 OG	2.5	H_2O 38	E211 OE1	2.4
β-Phosphate O2B	Mn^{2+}	2.1	H_2O 38	D213 OD1	2.8
GlcNAc O7	H_2O 263	2.8	H_2O 40	D212 OD2	3.0
GlcNAc O3	E211 OE1	2.7	H_2O 87	T315 OG1	3.0
GlcNAc O3	H2O 27	2.6	H_2O 116	G317 O	2.6
GlcNAc O4	E211 OE2	2.6	H_2O 263	D291 OD1	2.9
GlcNAc O4	W290 NE1	2.8	H_2O 263	R295 NH2	3.0

Tabl 8

Protein threading results. Proteins from different families were threaded against a THREADER 2 database containing 1900 protein folds, including GnT I, spsA, GlmU, and β4Gal-T1. The folds were sorted on the basis of their filtered combined energy Z-scores. When a GTCD-1-containing fold was one of the top thirty hits, out of 1900, then the top thirty hits were rerun with a randomization test of fifty shuffled-sequence threadings for each fold, to give a combined energy shuffled Z-score. A correct prediction should score well in both tests.

Family	Class	Protein (GenBank GI number)	Top GTCD-1-containing Hit	Z-score (rank)	Randomization Test Z-score (rank)
1	Inverting	*Petunia x hybrida* UDP-rhamnose anthocyanidin-3-glucosiderhamnosyltransferase (397567)	β4Gal-T1	2.33 (10)	3.28 (8)
2	Inverting	*H. influenzae* lgtD (1074167)	spsA	2.02 (2)	4.59 (1)
3	Retaining	*S. cerevisiae* Glycogen [Starch] Synthase, Isoform 1 (136753)	β4Gal-T1	2.90 (2)	4.47 (1)
4	Retaining	*Salmonella typhimurium* Lipopolysaccharide 1,2-N-acetylglusosaminetransferase rfaK (132488)	GlmU	2.63 (3)	3.81 (4)
		Shigella dysenteriae galactosyl-transferase RfpB (688322)	GlmU	2.61 (5)	0.52 (25)
5	Retaining	*Triticum aestivum* Granule-bound starch synthase (136765)	GlmU	2.41 (8)	0.72 (14)
6	Retaining	*Homo sapiens* histo-blood group A transferase (340077)	GlmU	3.09 (1)	2.28 (1)
		Synthetic blood group B alpha-1,3-galactosyltransferase (1041670)	GnT I / spsA	3.12 (1) / 2.63 (5)	3.47 (3) / 4.95 (1)
7	Inverting	*Lymnaea stagnalis* β-1,4-GlcNAc transferase	β4Gal-T1	14.98 (1)	11.75 (1)
8	Retaining	*Oryctolagus cuniculus* Glycogenin-1 (417075)	GnT I	2.48 (5)	3.49 (1)
9	Inverting	*Bordetella pertussis* rfaC (992970)	GlmU	2.59 (6)	1.31 (19)
10	Inverting	*Homo sapiens* Fucosyltransferase 5 (1730135)	GlmU	2.90 (1)	1.60 (16)
11	Inverting	*Homo sapiens* Fucosyltransferase 1 (120636)	GlmU	3.46 (1)	1.73 (14)
12	Inverting	*Homo sapiens* GM2/GD2 synthase (1168736)	GlmU	2.80 (2)	1.24 (10)
13	Inverting	*C. elegans* gly-14 (3420844)	GnT I	20.26 (1)	12.34 (1)
14	Inverting	*Homo sapiens* Core2 GlcNAc-transferase (544360)	spsA	3.13 (4)	5.05 (1)
15	Retaining	*Candida albicans* putative mannosyltransferase Mnt1 (1480086)	spsA	2.37 (13)	1.74 (10)
16	Inverting	*Homo sapiens* GnT II (1708004)	spsA	2.84 (2)	4.53 (1)
17	Inverting	*Homo sapiens* GnT III (1169979)	GlmU	2.85 (2)	0.66 (15)
18	Inverting	*Homo sapiens* GnT V (1169980)	GlmU / GnT I	2.82 (2) / 2.52 (7)	2.33 (6) / 2.41 (4)
19	???	*E. coli* lipid A disaccharide synthase (126464)	GlmU	2.72 (5)	0.86 (15)
20	Retaining	*A. thaliana* trehalose-6-phosphate synthase (1865676)	GlmU	2.94 (3)	1.48 (9)
21	Retaining	*Homo sapiens* ceramide glucosyltransferase (2498228)	GlmU	2.81 (1)	1.08 (9)
22	???	*Homo sapiens* PIG-B (1552168)	GlmU	2.64 (3)	0.14 (27)
23	Inverting	*Sus scrofa* N-acetyl-β-D-glucosaminide α-1,6-fucosyltransferase (1752753)	GlmU	2.33 (8)	0.85 (16)
24	Retaining	*Drosophila melanogaster* UDP-glucose glycoprotein glucosyltransferase (790584)	GlmU / GnT I / spsA	3.54 (1) / 3.05 (3) / 2.82 (7)	1.84 (2) / 1.74 (3) / 2.03 (1)
		Saccharomyces cerevisiae Killer-toxin resistance protein 5 precursor (2507054)	GlmU / spsA	3.05 (2) / 2.99 (3)	2.23 (5) / 5.39 (1)
25	Inverting	*Haemophilus influenzae* Lipooligosaccharide biosynthesis protein lex-1 (1170778)	SpsA	2.39 (8)	1.51 (2)
26	???	*Bacillus subtilis* Teichoic acid biosynthesis protein A (135271)	GlmU	3.57 (1)	7.42 (1)
27	Retaining	*Homo sapiens* polypeptide N-acetylgalactosaminyltransferase (1709558)	GlmU / β4Gal-T1 / GnT I / spsA	3.06 (2) / 2.96 (3) / 2.94 (4) / 2.48 (12)	1.75 (14) / 3.19 (4) / 4.34 (2) / 2.38 (10)

WE CLAIM:

1. A secondary or three-dimensional structure of a purified glycosyltransferase when it associates with a nucleotide sugar donor, acceptor, or metal cofactor.
2. A secondary or three-dimensional structure of a purified glycosyltransferase in association with a moiety.
3. A secondary or three-dimensional structure as claimed in claim 2, wherein the moiety is a nucleotide sugar donor, acceptor, metal cofactor, or heavy metal atom.
4. A secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims that is a crystalline form.
5. A secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims, wherein the glycosyltransferase is an N-acetylglucosaminyltransferase.
6. A secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims having one or both of the following characteristics:
   (a) an N-terminal domain comprising an eight-stranded mixed β-sheet flanked by six helices, and a small two-stranded antiparallel β-sheet ; and
   (b) a C-terminal domain comprising a four-stranded mixed β-sheet flanked by three α-helices and a short β-finger.
7. A secondary or three-dimensional structure of a glycosyltransferase as defined in claim 6 further characterized by the N-terminal domain and C-terminal domain being connected by a linker region which wraps halfway around the N-terminal domain before starting the first helix of the C-terminal domain.
8. A secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims having the structural coordinates of a glycosyltransferase listed in Table 1, 2, 3, or 4.
9. A secondary or three-dimensional structure of a glycosyltransferase in association with a sugar nucleotide donor having the structural coordinates of a glycosyltransferase and a sugar nucleotide donor listed in Table 3.
10. A secondary or three-dimensional structure of a glycosyltransferase in association with an acceptor having the structural coordinates of a glycosyltransferase and an acceptor listed in Table 4.
11. A crystalline form of a glycosyltransferase having a unit cell with dimensions of a = 40.4 ± 3 Å, b=82.4 ± 3 Å, and c = 102.5 ± 3 Å.
12. A crystalline form of an N-acetylglucosaminyltransferase having the structural coordinates listed in Table 1, 2, 3, or 4, and a unit cell with dimensions of a = 40.4 ± 3 Å, b=82.4 ± 3 Å, and c = 102.5 ± 3 Å.
13. A crystalline form as claimed in claim 11 or 12 further characterized by the parameters, diffraction statistics, and/or refinement statistics in Table 6.

14. A secondary or three-dimensional structure of a binding site of a secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims.
15. A secondary or three-dimensional structure of a binding site as claimed in claim 14 wherein the binding site is defined by its association with one or more of a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a sugar of a nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, and/or an acceptor.
16. A secondary or three-dimensional structure of a binding site of a glycosyltransferase as defined in the preceding claims wherein the binding site is also defined by the atomic interactions of Table 5, preferably the enzyme atomic contacts.
17. A secondary or three-dimensional structure of a binding site of a glycosyltransferase as defined in the preceding claims wherein the binding site is defined by atomic interactions 1 to 5; 6 and 7; 8, 9 and 10; 1 to 13; 14 to 21; 22 to 27; 1 to 13; 1 to 21; or 11, 12, 13, and 27 listed in Table 5, or the enzyme atomic contacts for these atomic interactions listed in Table 5.
18. A secondary or three-dimensional structure of an spsA GnT 1 core (SGC) domain of a secondary or three-dimensional structure of a glycosyltransferase as defined in any of the preceding claims.
19. A secondary or three-dimensional structure of an SGC domain as claimed in claim 18 characterized by an eight-stranded mixed β-sheet, flanked by six helices, and a small two-stranded antiparallel β-sheet.
20. A modulator of the activity of a glycosyltransferase derived from a secondary or three-dimensional structure as claimed in any of the preceding claims.
21. A method of determining three-dimensional structures of polypeptides with unknown structure comprising the step of applying the structural coordinates of Table 1, 2, 3, or 4.
22. A method for identifying a potential modulator of a glycosyltransferase, or binding sites or domains thereof, comprising the step of using the structural coordinates of Table 1, 2, 3, or 4 that define a glycosyltransferase or binding sites or domains thereof, to computationally evaluate a test compound for its ability to associate with the glycosyltransferase, binding sites or domains thereof, wherein a test compound that associates is a potential modulator of a glycosyltransferase.
23. A method for identifying a modulator of a glycosyltransferase by determining binding interactions between a test compound and secondary or three-dimensional structures of binding sites as defined in any of the preceding claims comprising:

    (a) generating the binding sites on a computer screen;

    (b) generating a test compound with its spatial structure on the computer screen; and

    (c) testing to determine whether the test compound binds to a selected number of binding sites.
24. A method for identifying a potential modulator of a glycosyltransferase function comprising the steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of a secondary or three-dimensional structure of a glycosyltransferase or a binding site as defined in any of the preceding claims, to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying compounds that best fit the selected site as potential modulators of the glycosyltransferase.

25. A method for identifying a potential modulator of a glycosyltransferase function comprising the steps:

(a) modifying a computer representation of a compound complexed with a secondary or three-dimensional structure of a glycosyltransferase or a binding site as defined in any of the preceding claims, by deleting or adding a chemical group or groups;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying a compound that best fits the binding cavity as a potential modulator of a glycosyltransferase.

26. A method for identifying a potential modulator of a glycosyltransferase function comprising the steps:

(a) selecting a computer representation of a compound complexed with a secondary or three-dimensional structure of a glycosyltransferase or a binding site as defined in any of the preceding claims; and

(b) searching for molecules in a data base that are similar to the compound using a searching computer program, or replacing portions of the compound with similar chemical structures from a data base using a compound building computer program.

27. A modulator of a glycosyltransferase identified by a method as claimed in any of the preceding claims.

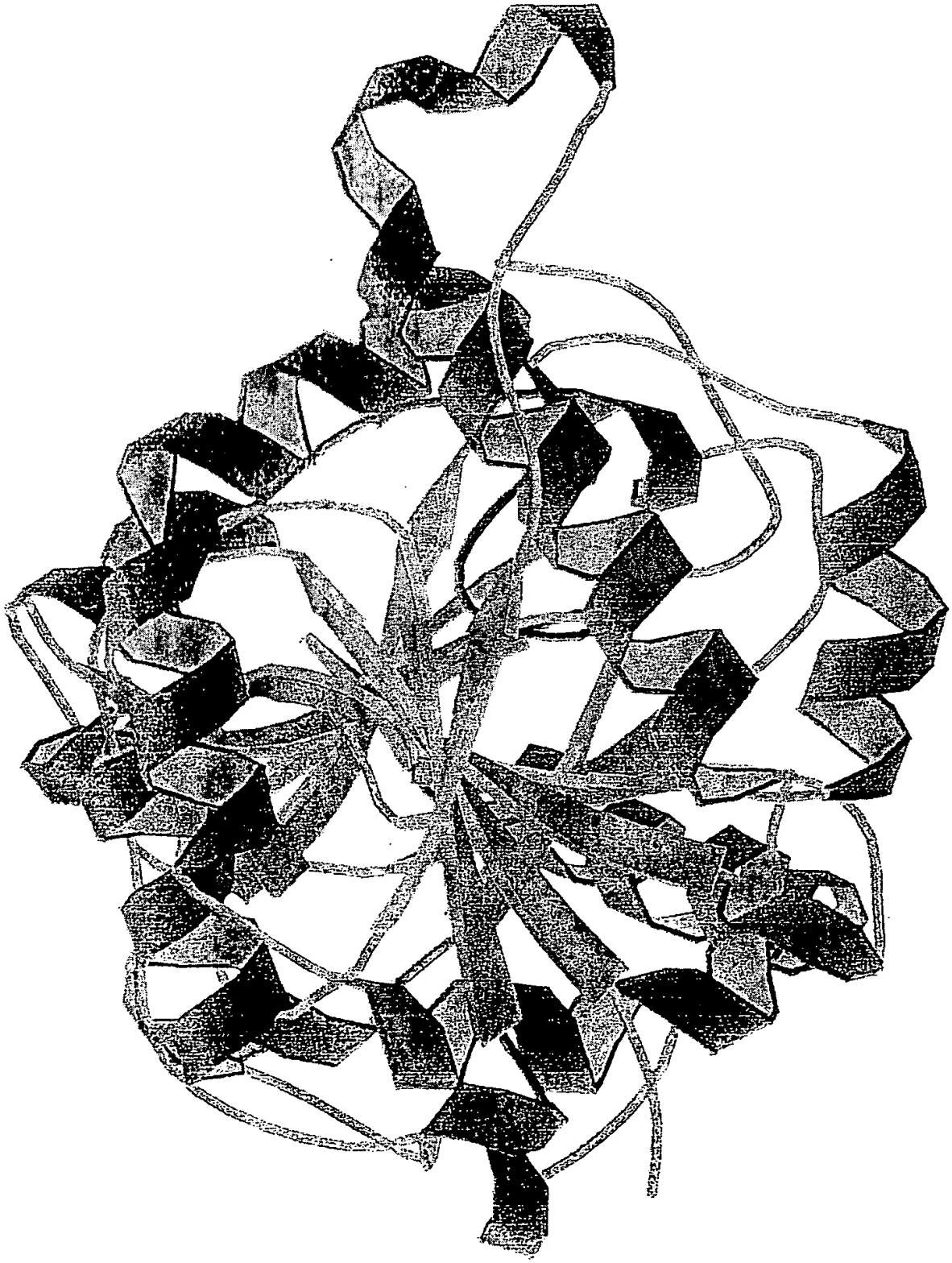
28. A method for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of a sugar nucleotide donor or acceptor or component thereof, defined in relation to it spatial association with the three dimensional structure of a glycosyltransferase or a binding site as defined in any of the preceding claims, to generate a compound that is capable of associating with the glycosyltransferase or binding cavity thereof.

29. A modulator of a glycosyltransferase based on a three-dimensional structure of a sugar nucleotide donor, an acceptor, or a component thereof, defined in relation to the sugar nucleotide donor's or acceptor's spatial association with a secondary or three-dimensional structure of a glycosyltransferase or binding site as defined in the preceding claims.

30. A pharmaceutical composition comprising a modulator as claimed in any of the preceding claims either alone or with other active substances.

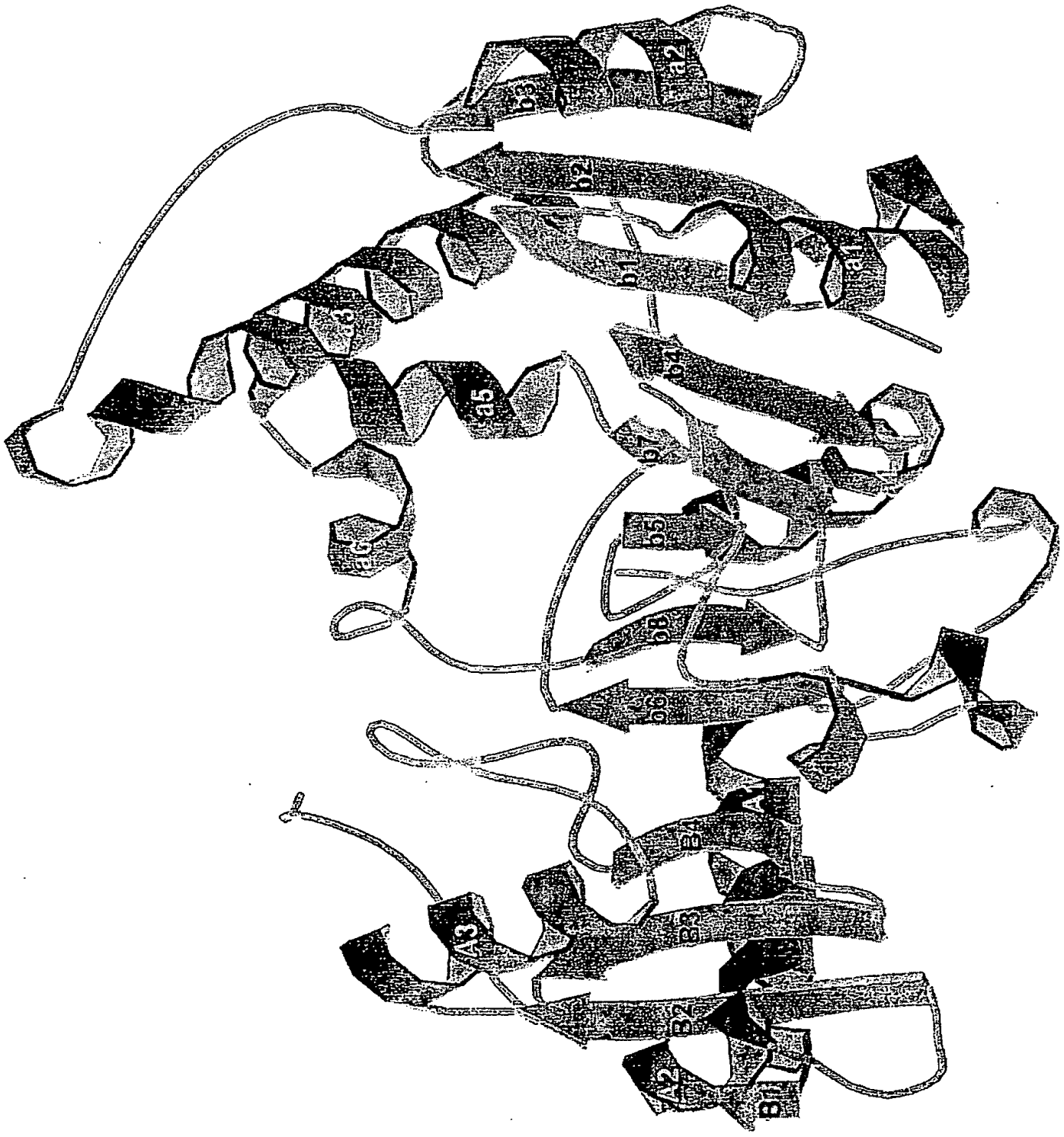
31. A method of treating a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism, comprising:
    (a) administering a pharmaceutical composition as claimed in claim 30; and
    (b) activating or inhibiting a glycosyltransferase to treat the disease.
32. Use of a modulator identified by the methods of any of the preceding claims in the preparation of a medicament to treat a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism.
33. Use of structural coordinates of a glycosyltransferase structure as set out in Table 1, 2, 3, or 4 to manufacture a medicament.
34. Machine readable media encoded with data representing the structural coordinates of a secondary or three-dimensional structure of a glycosyltransferase or a binding site as defined in any of the preceding claims.
35. A machine readable media as claimed in claim 34 wherein the data also includes structural coordinates for a nucleotide sugar donor, acceptor, metal cofactor, or heavy metal atom.

Figure 1



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Figure 2



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Figure 3

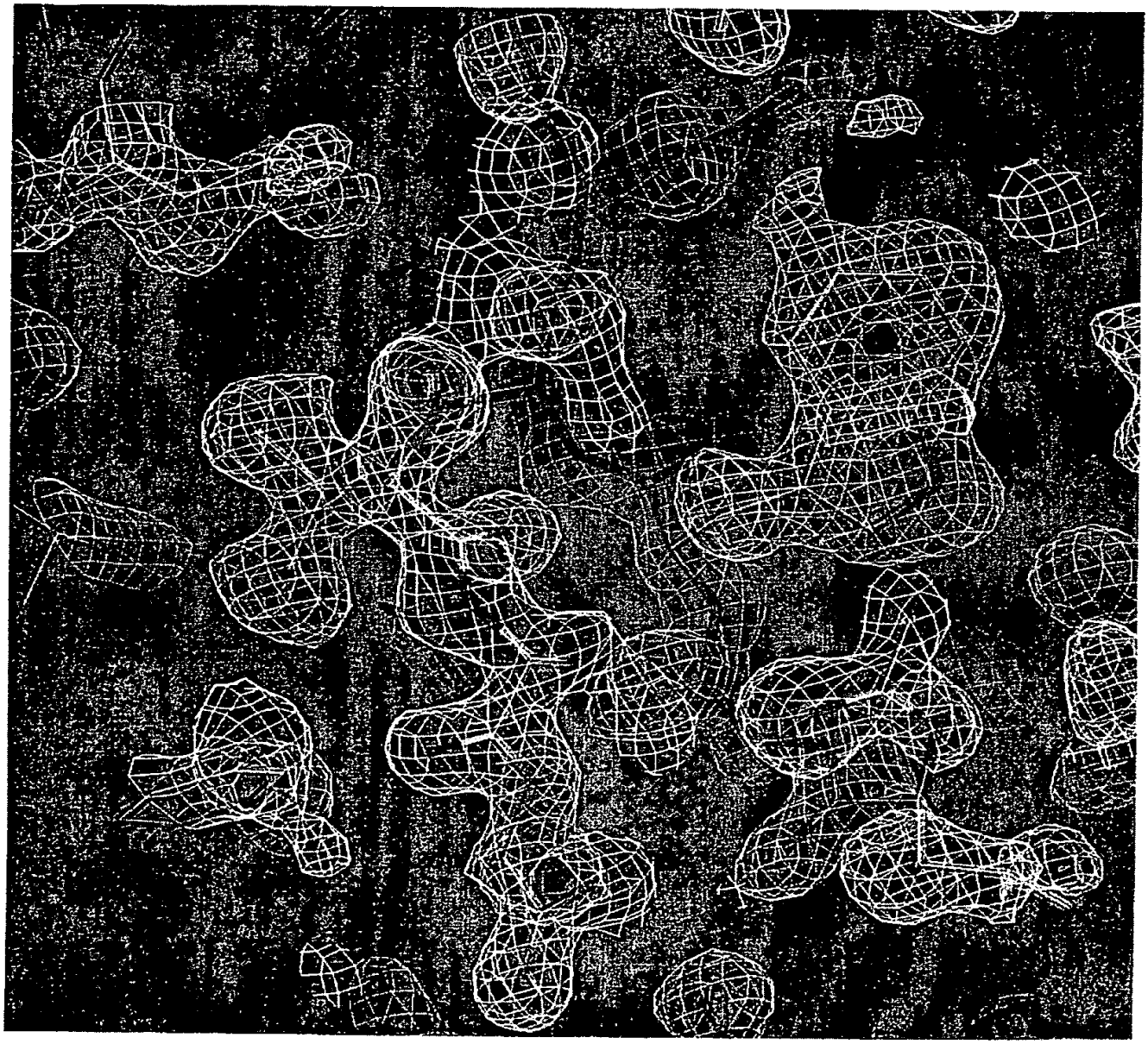


Figure 4

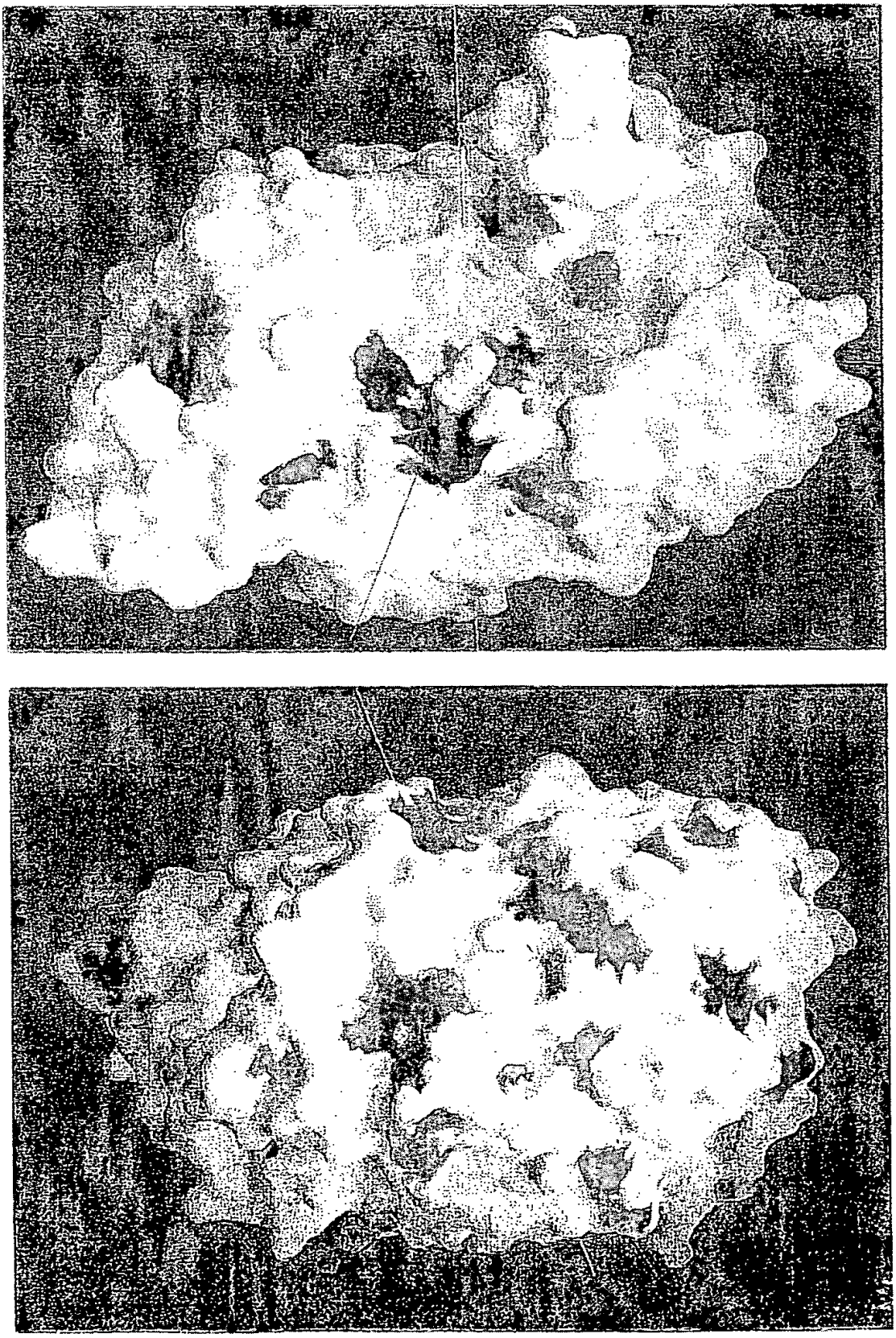
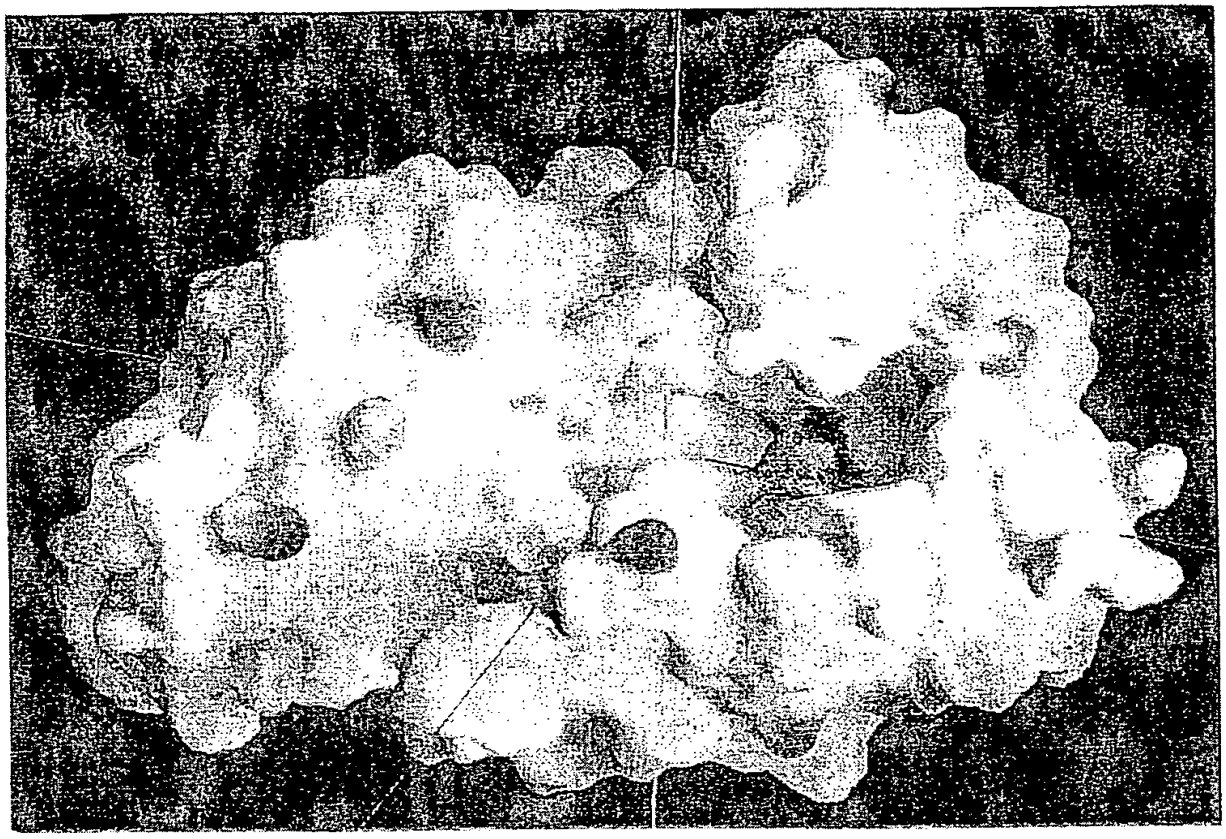


Figure 5



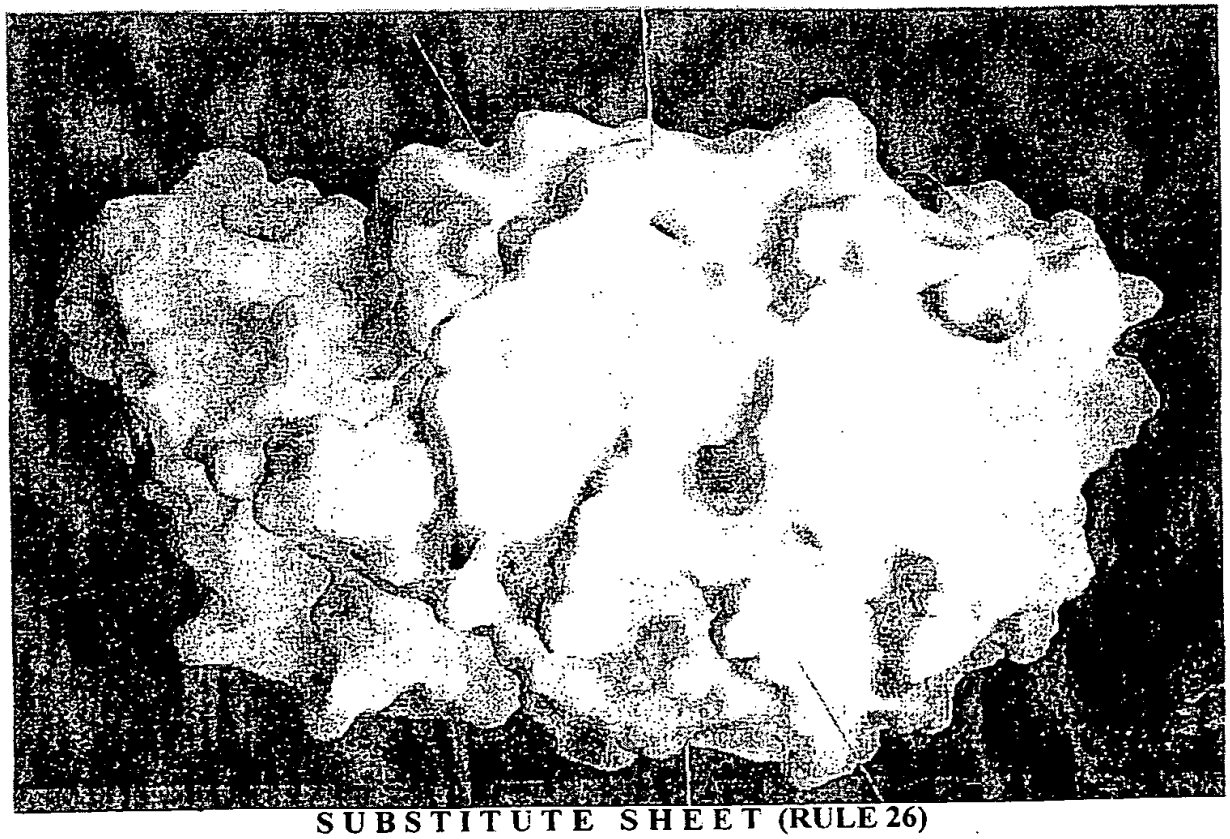


Figure 6



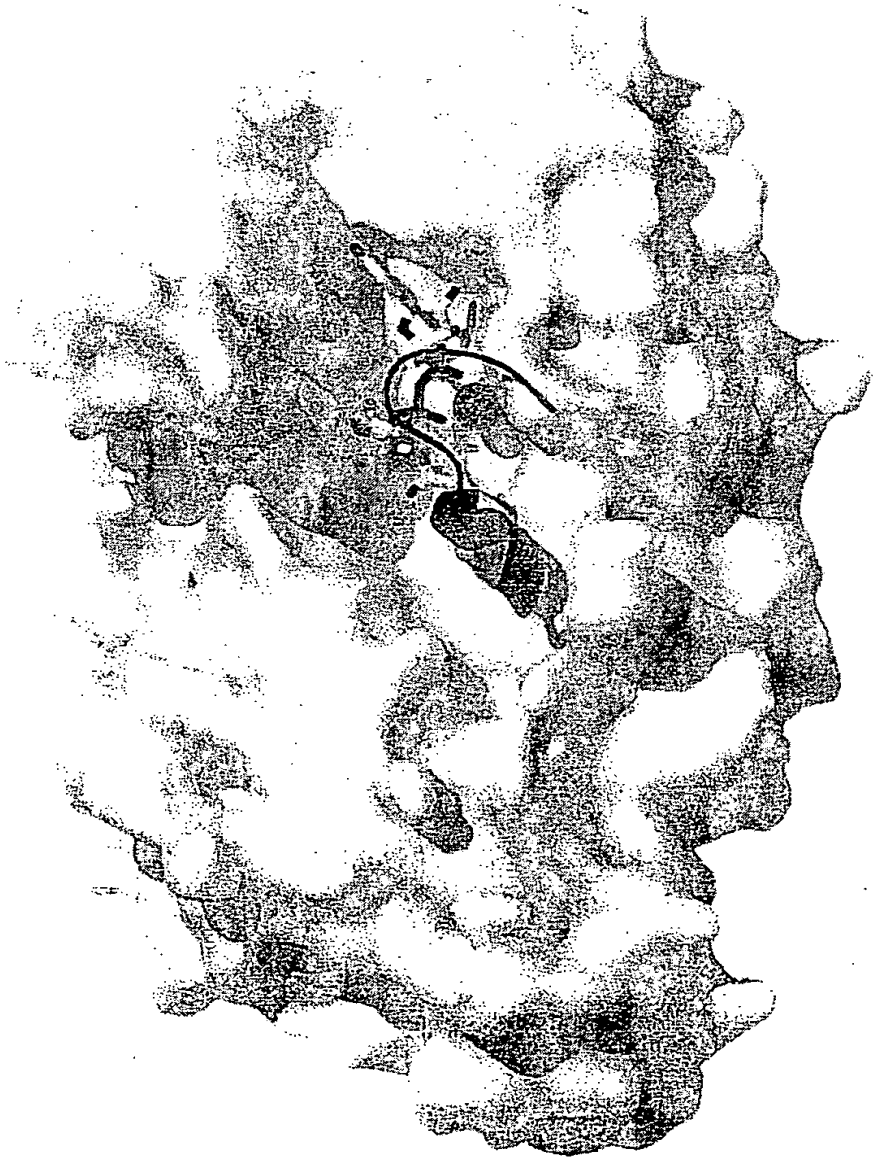
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Figure 7



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Figure 8A



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Figure 8B



Figure 8C

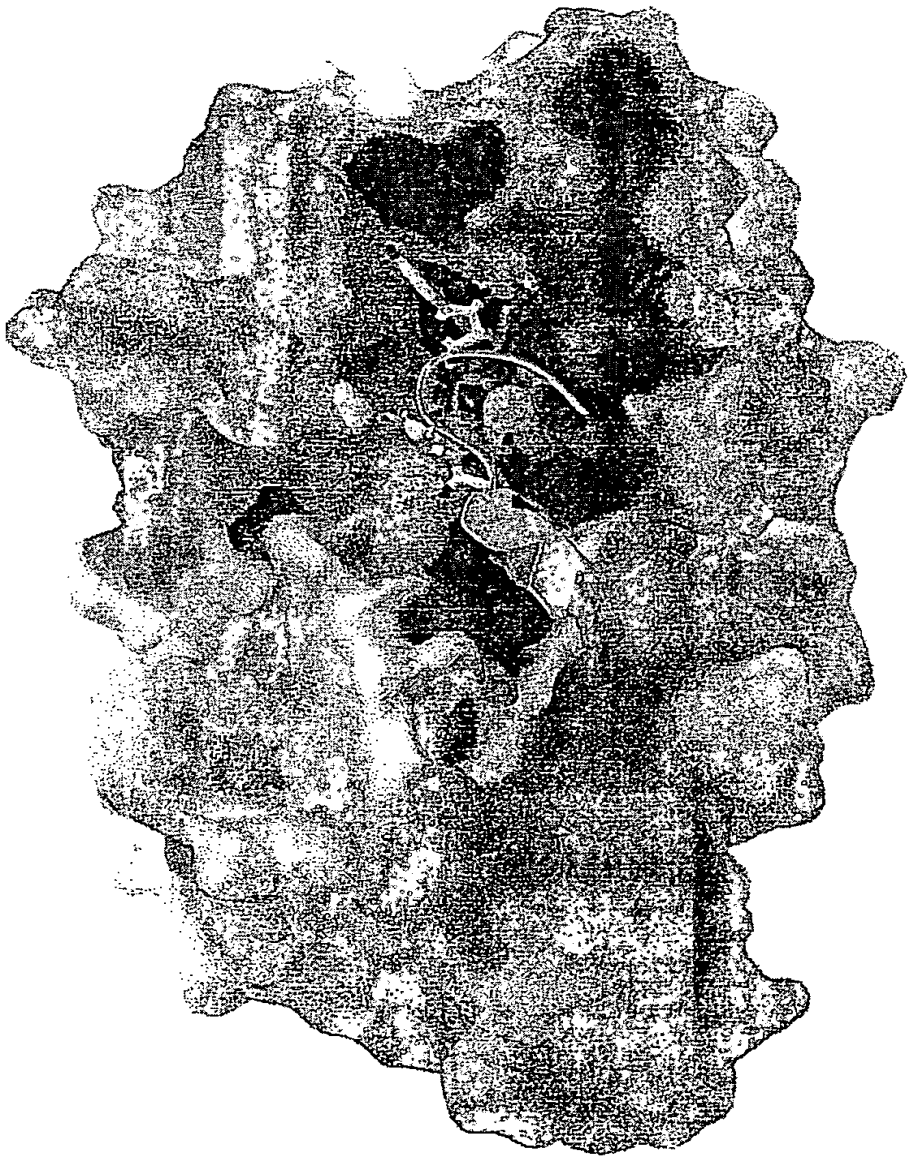
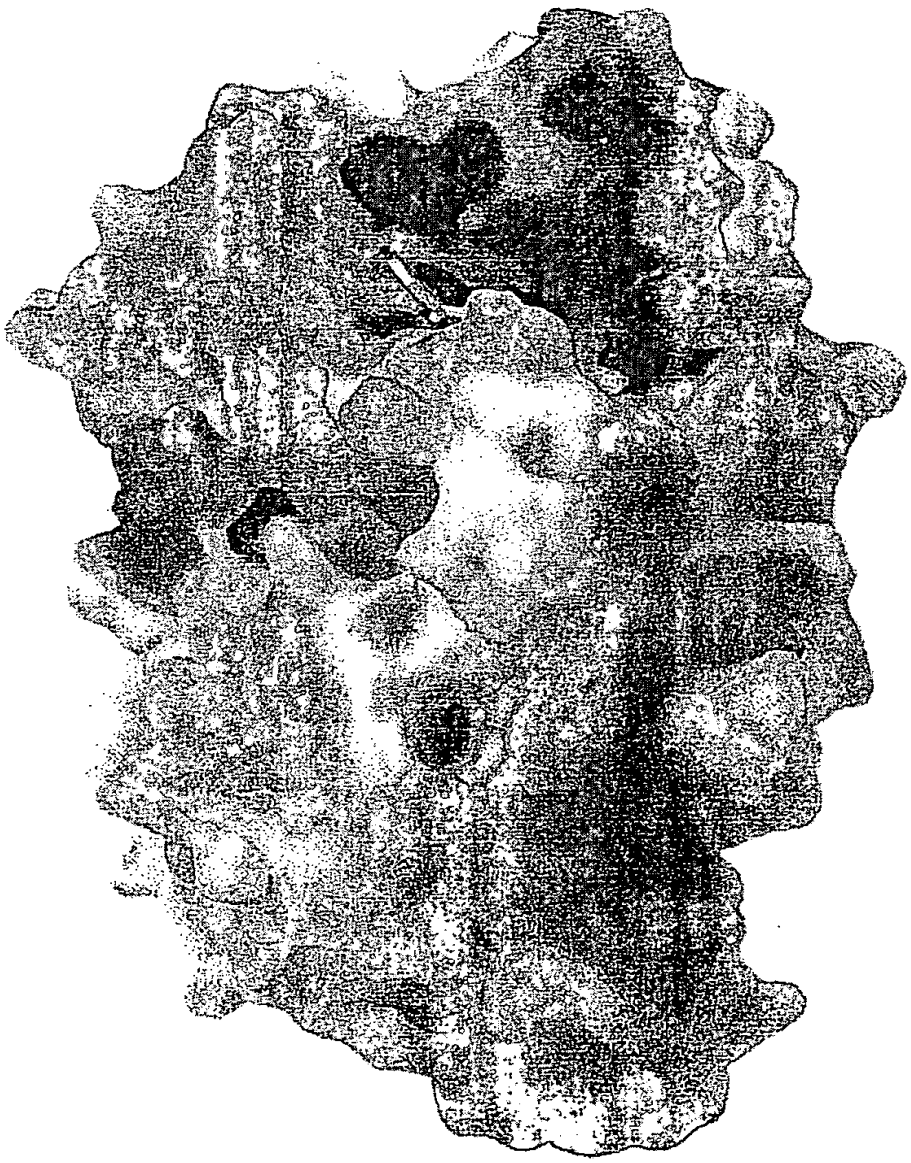


Figure 8D



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Figure 8E

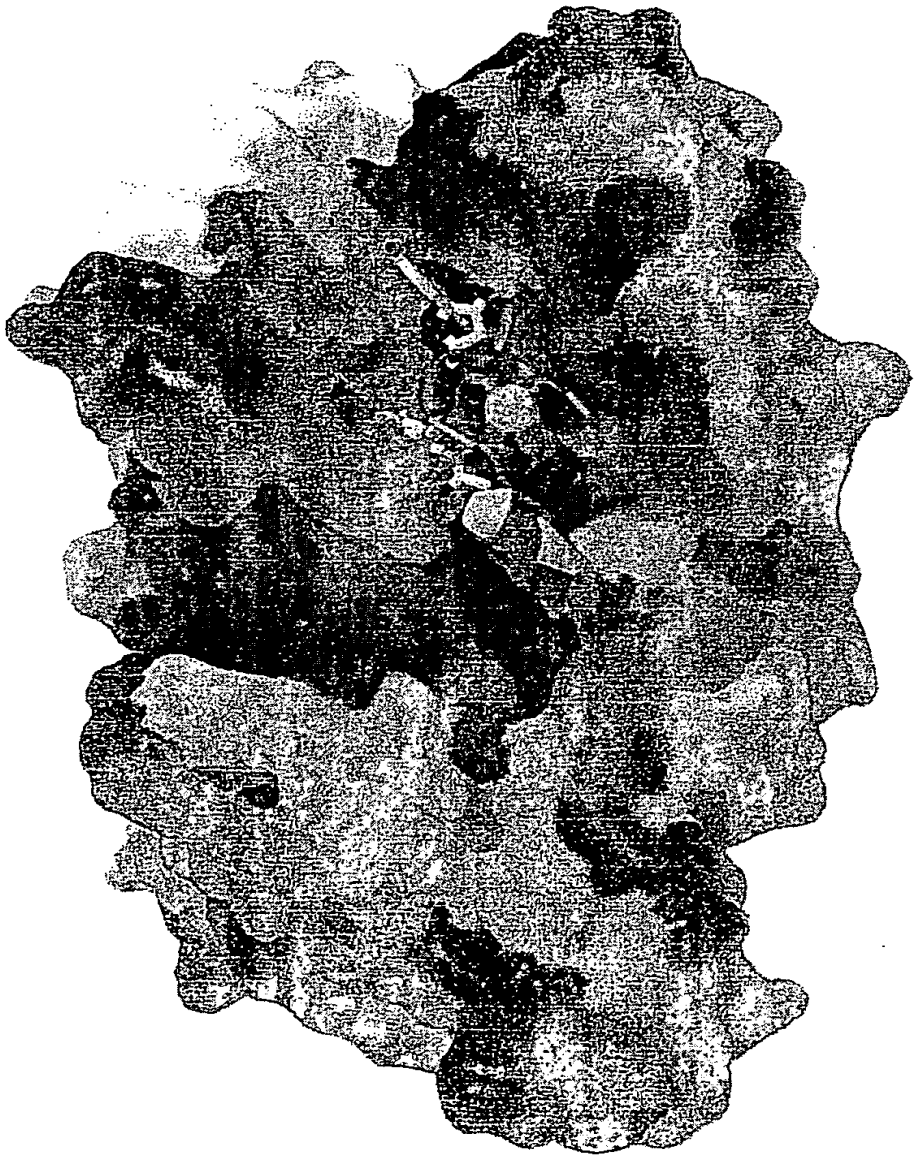


Figure 8F

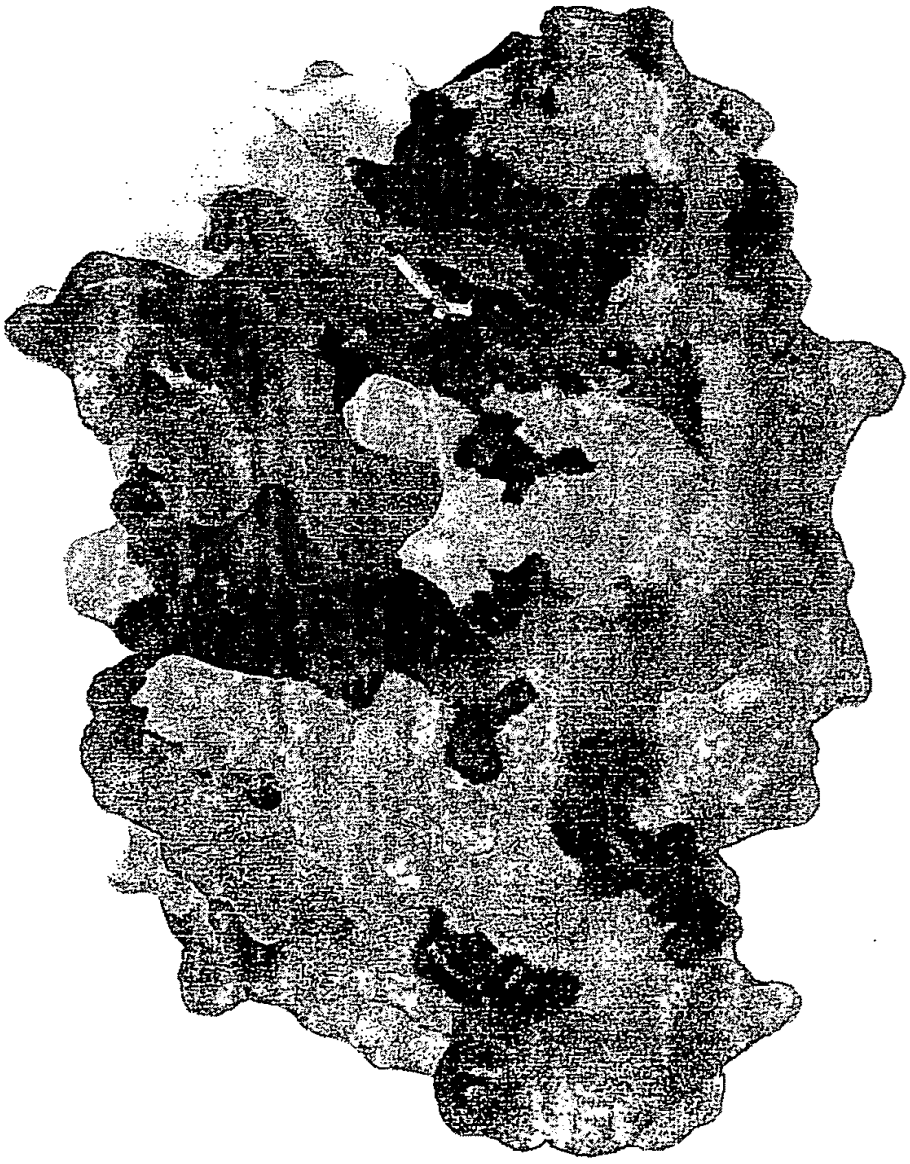


Figure 9A

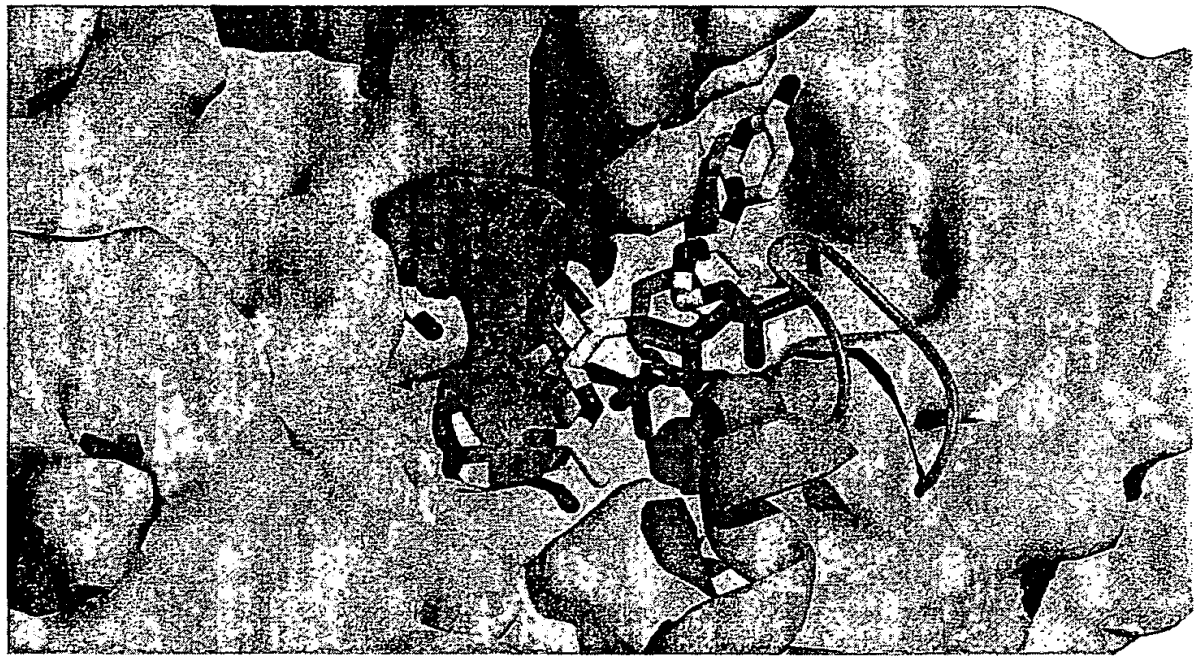


Figure 9B



Figure 10A

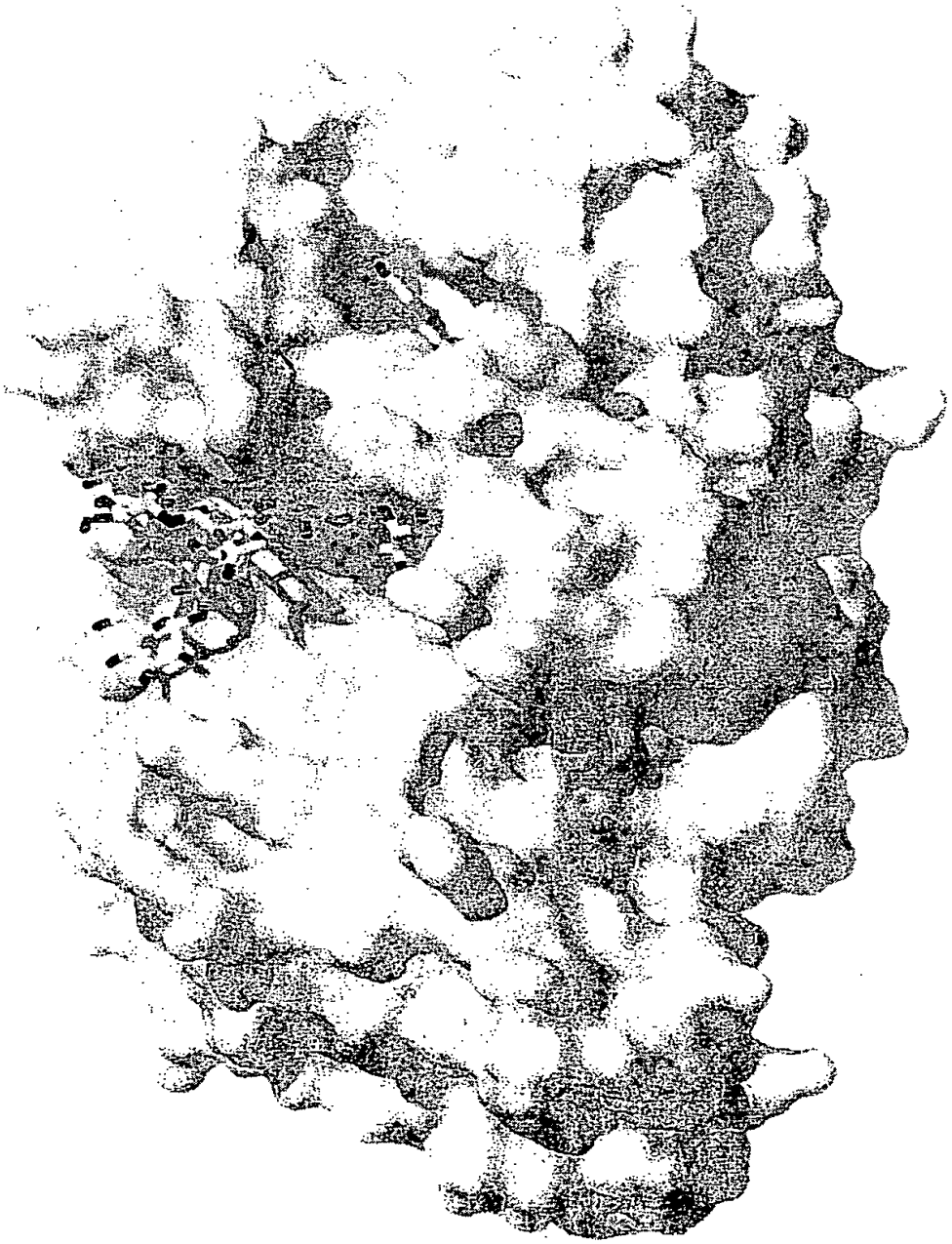


Figure 10B

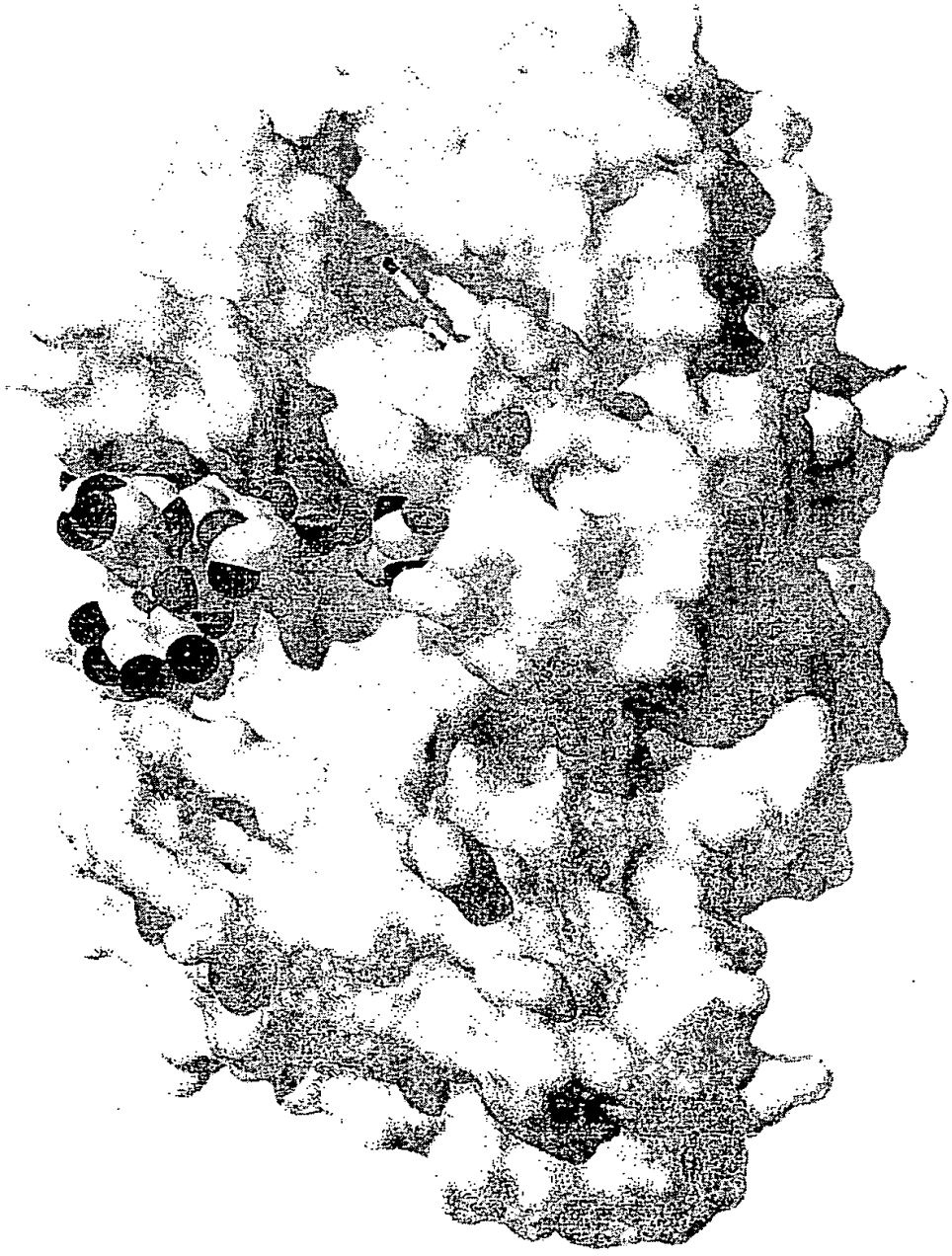


Figure 11A



Figure 11B

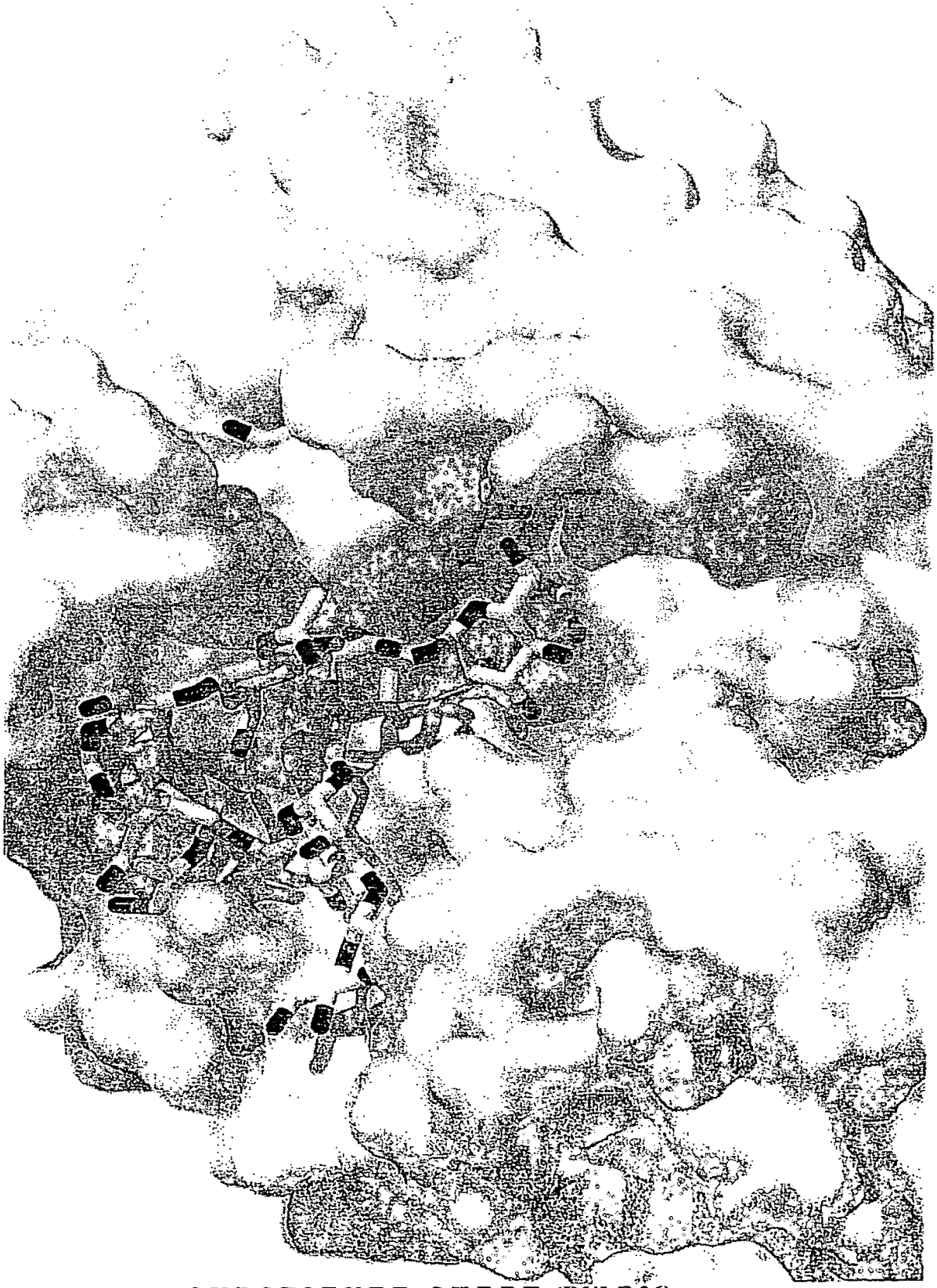


Figure 11C

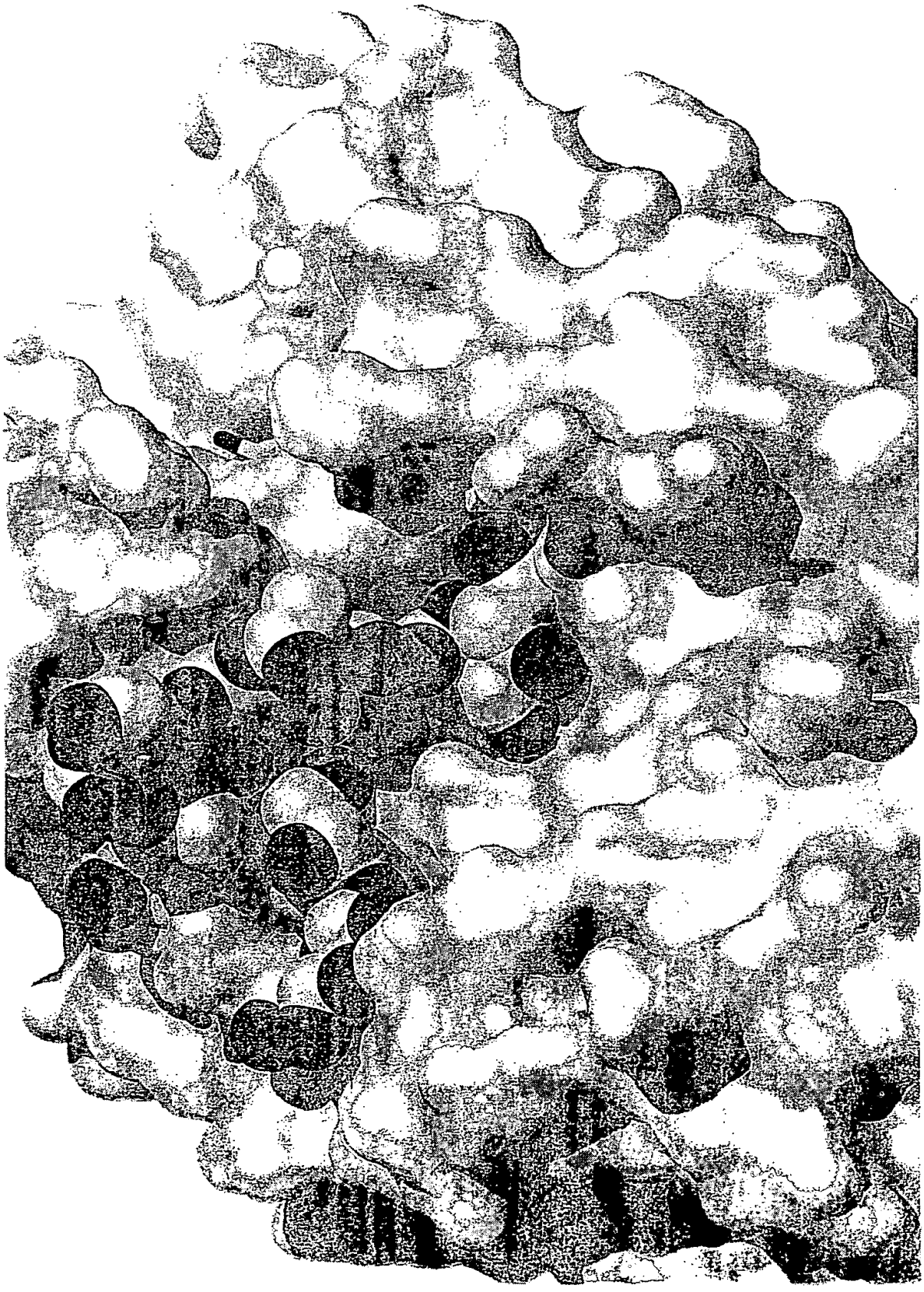


Figure 11D

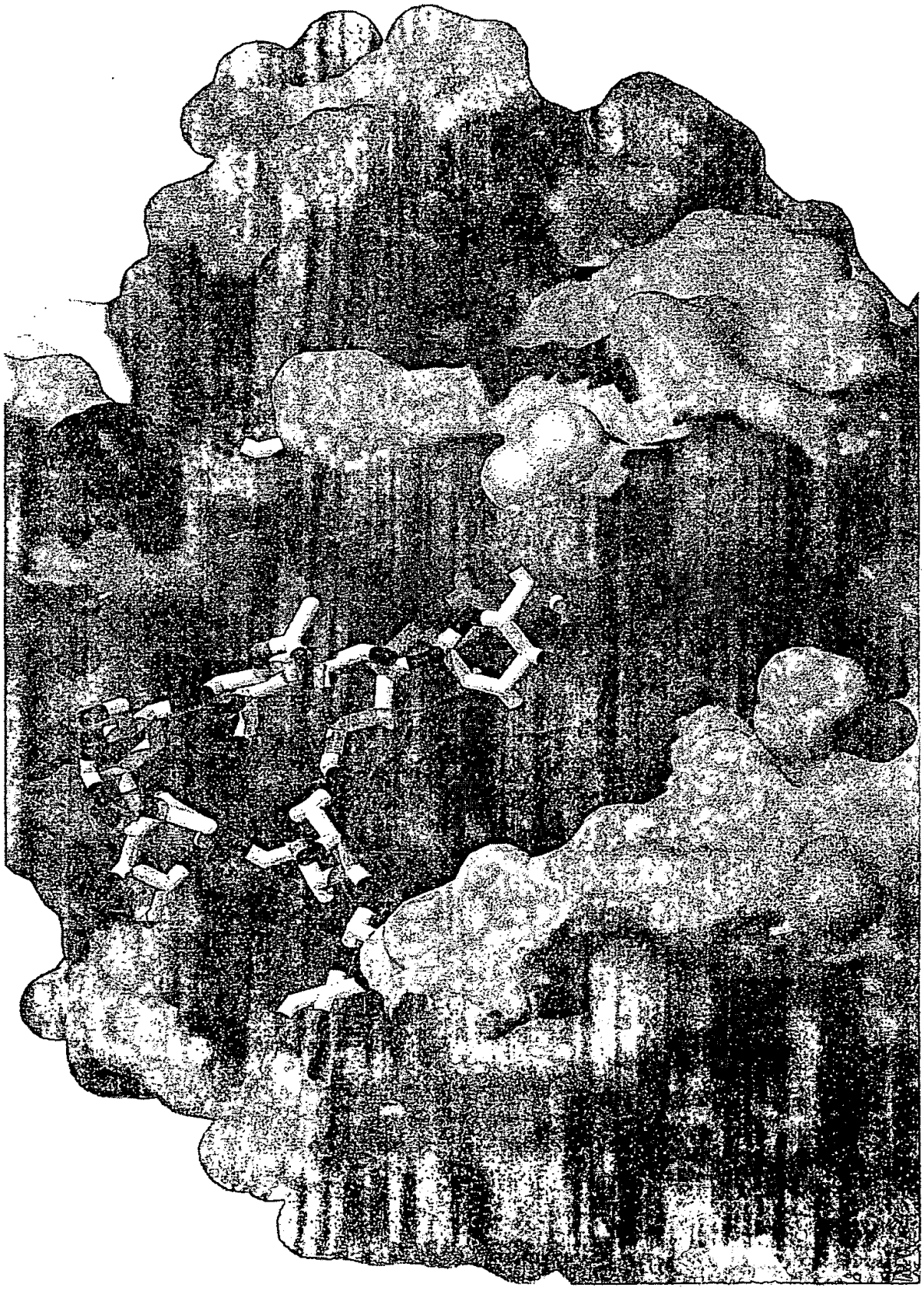


Figure 12

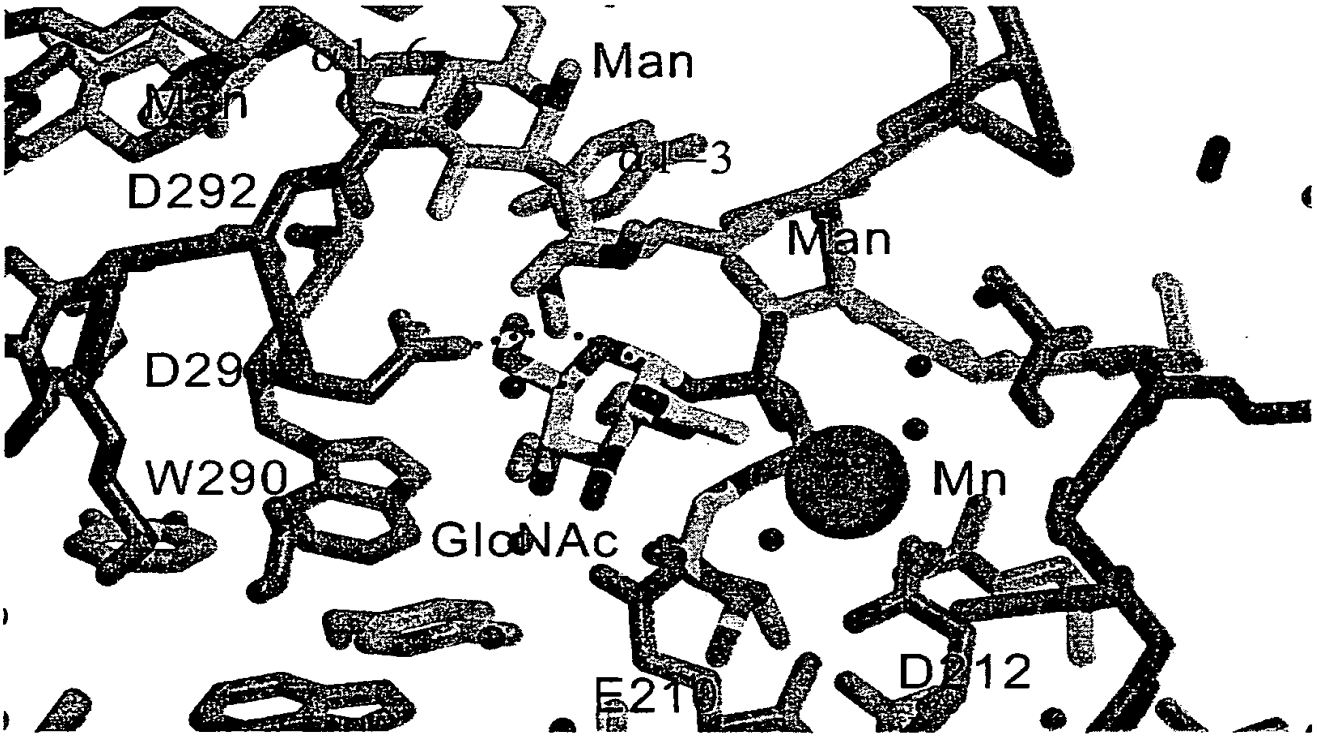


Figure 13

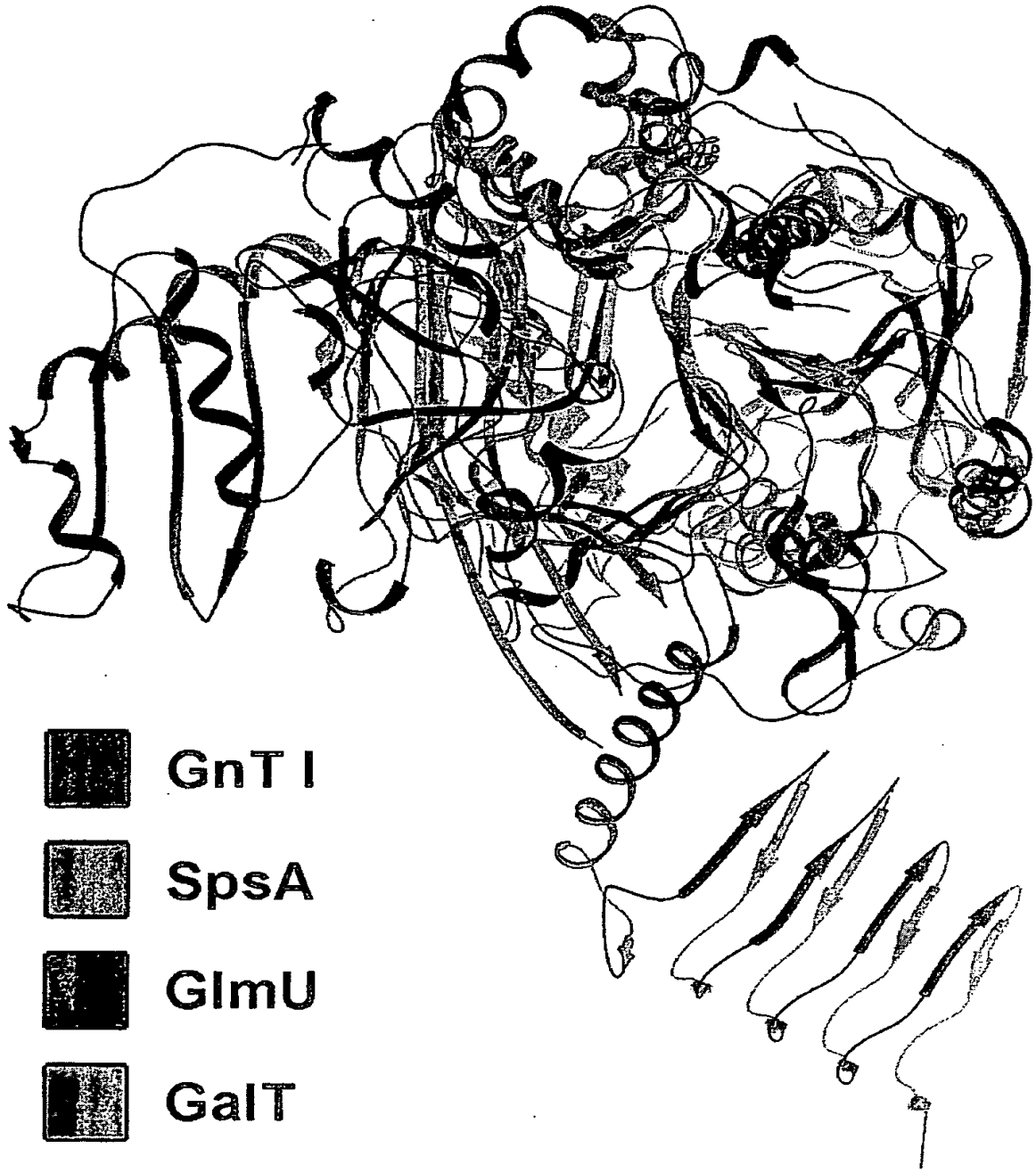
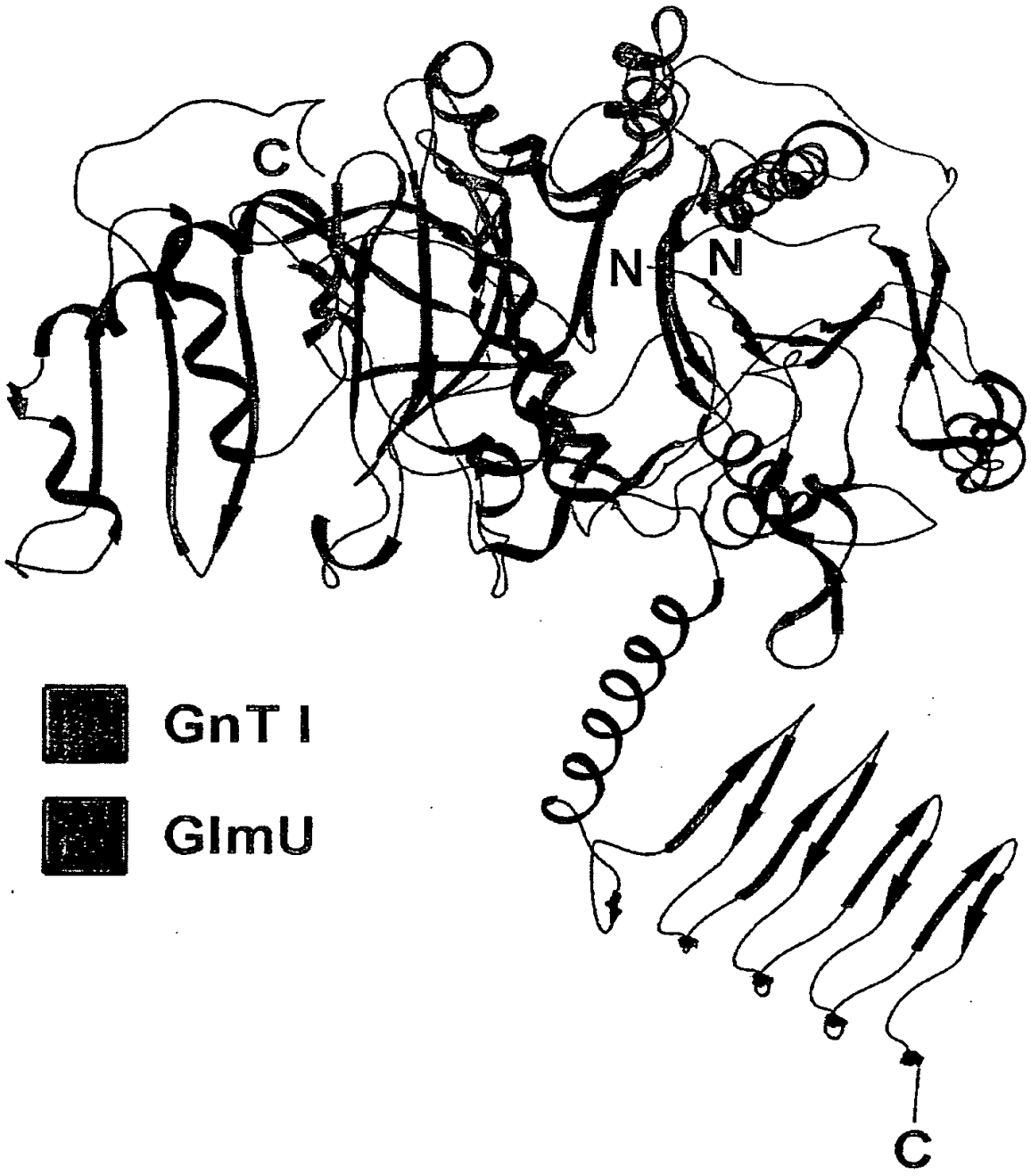


Figure 14



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Figure 15



Figure 16

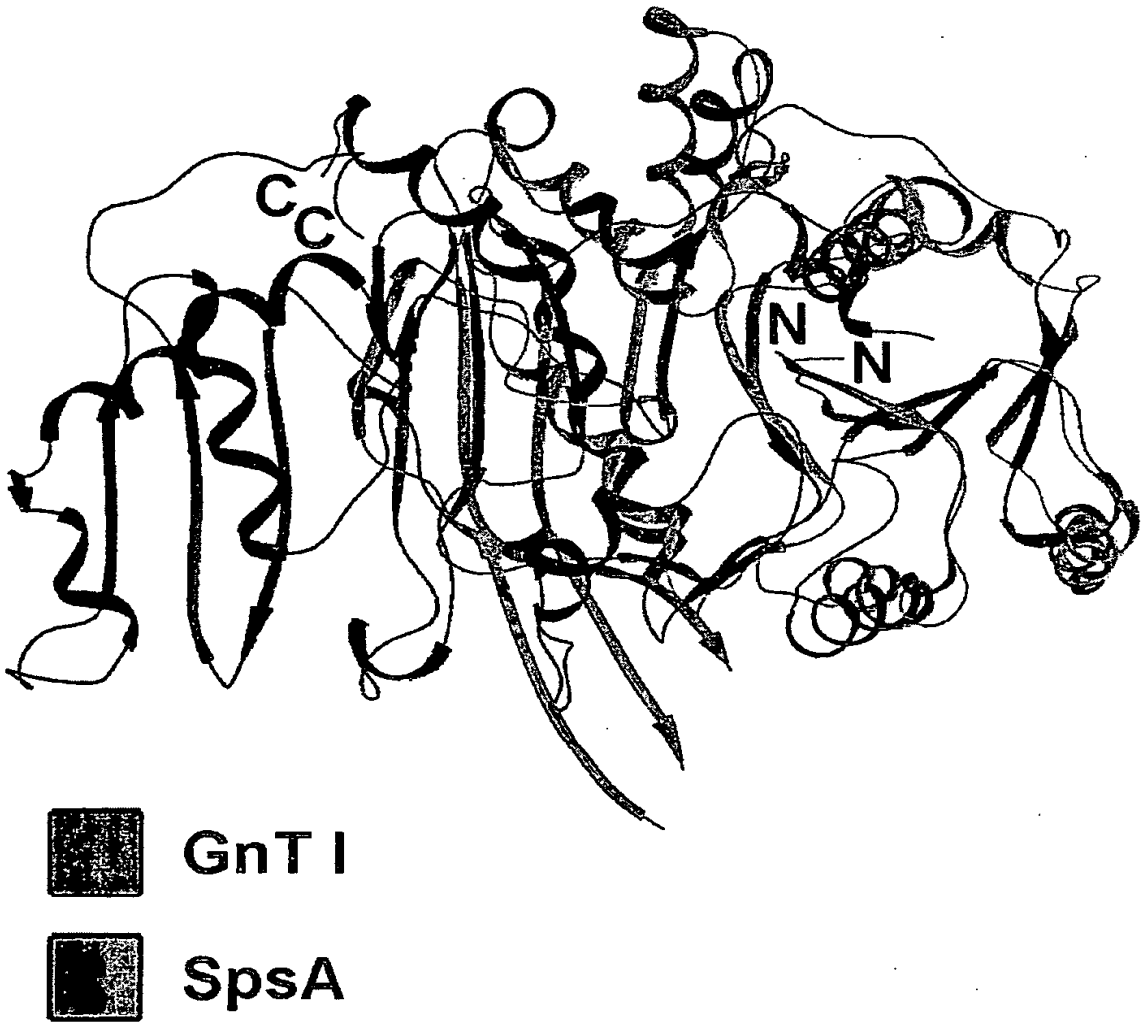
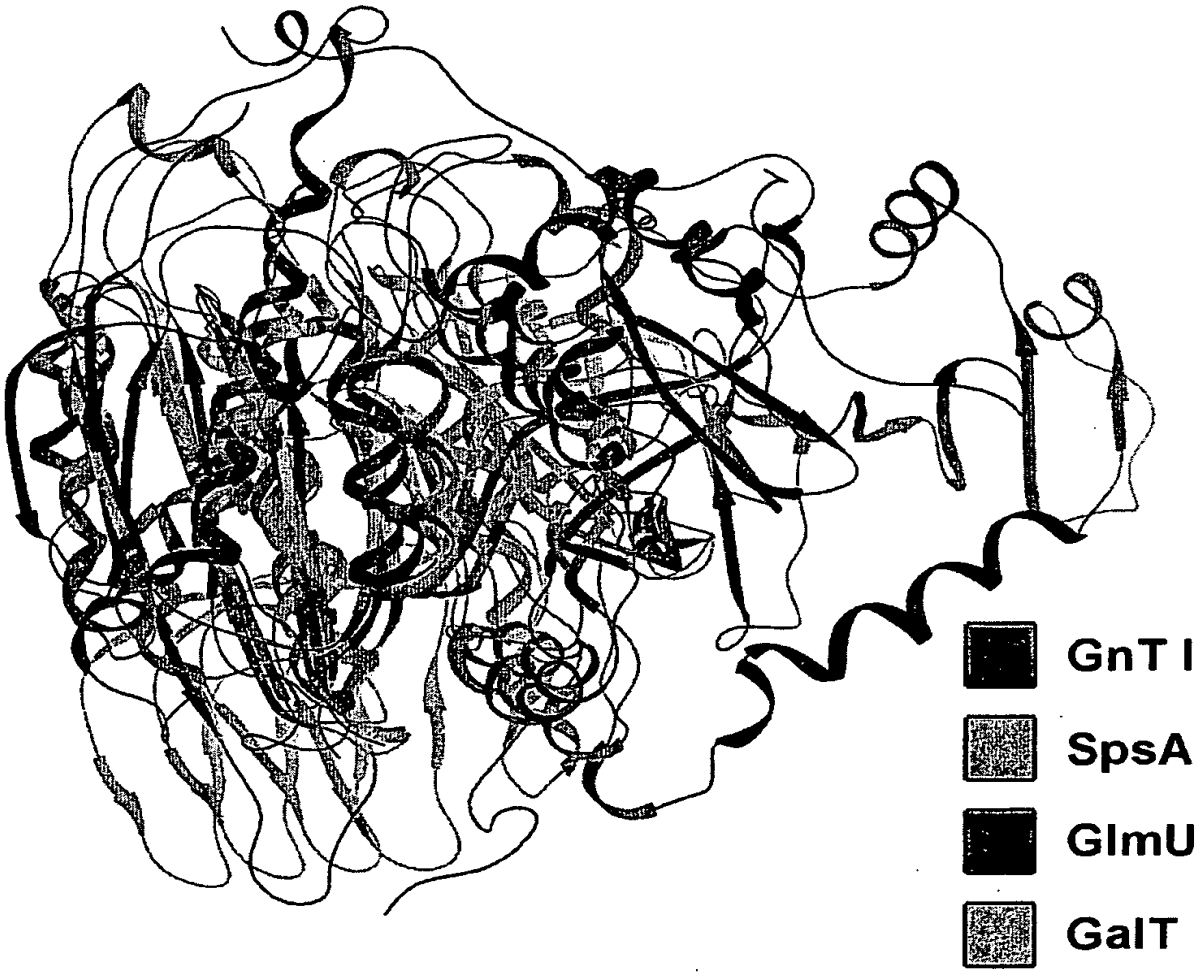
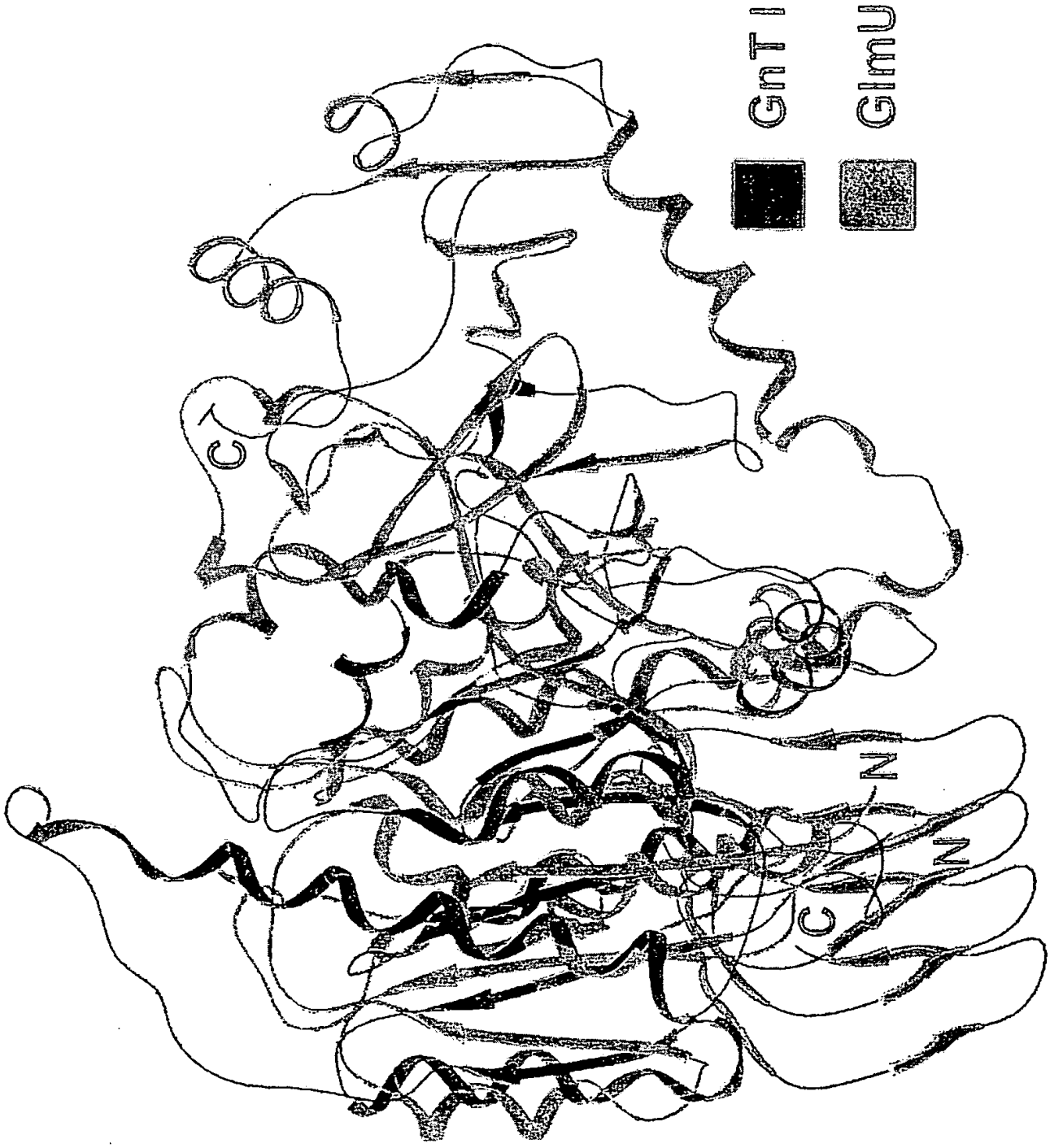


Figure 17



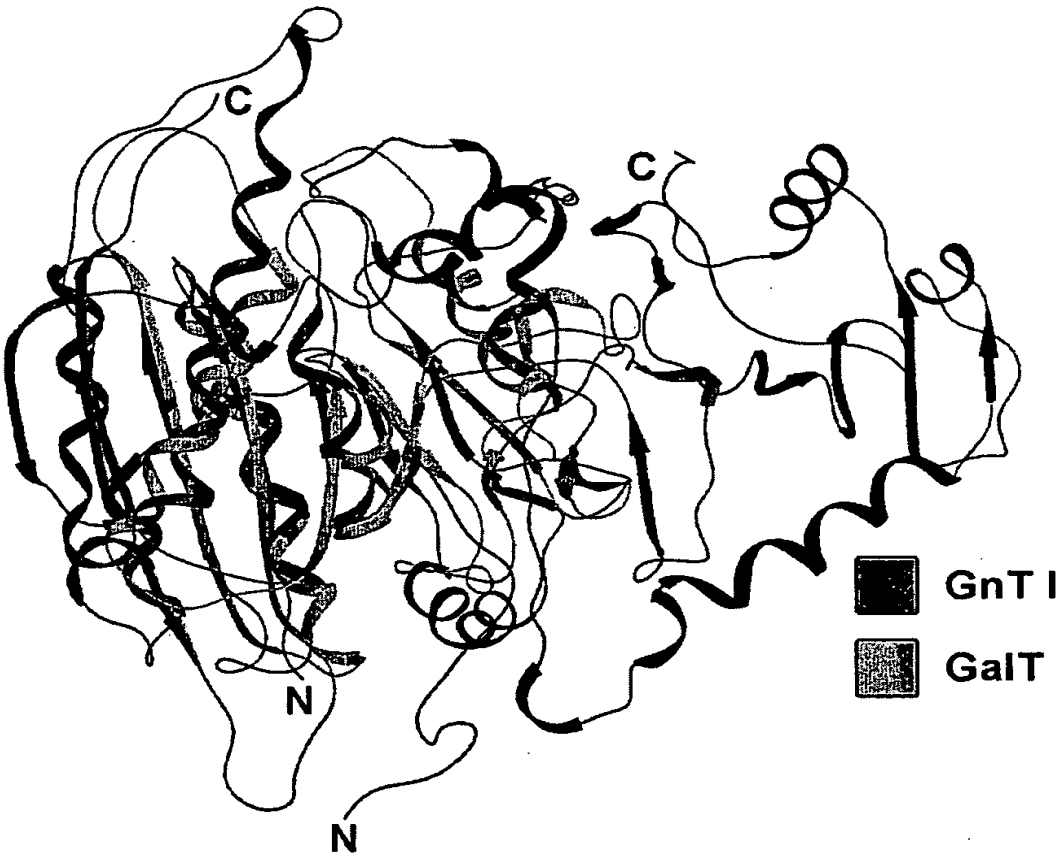
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Figure 18



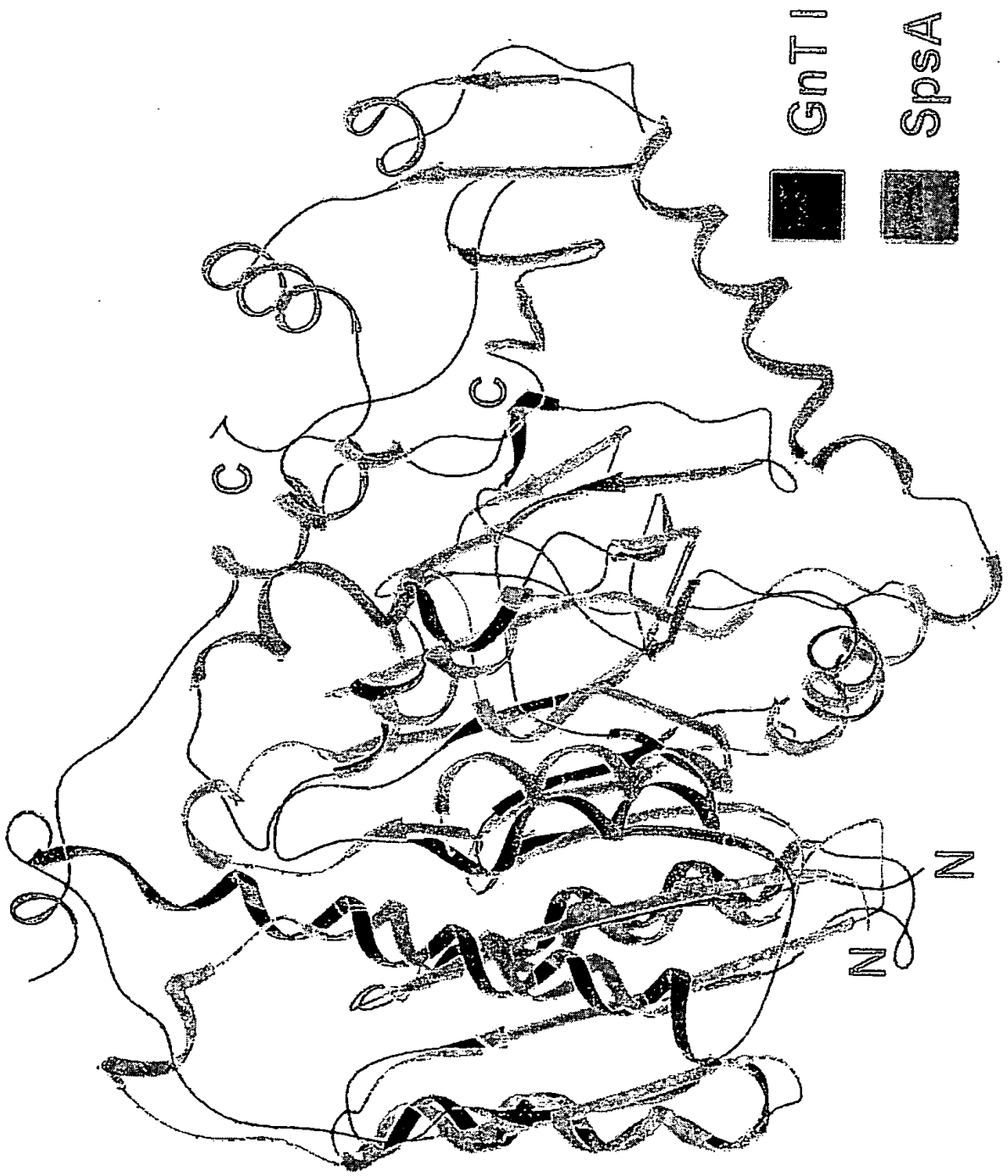
29/53

Figure 19



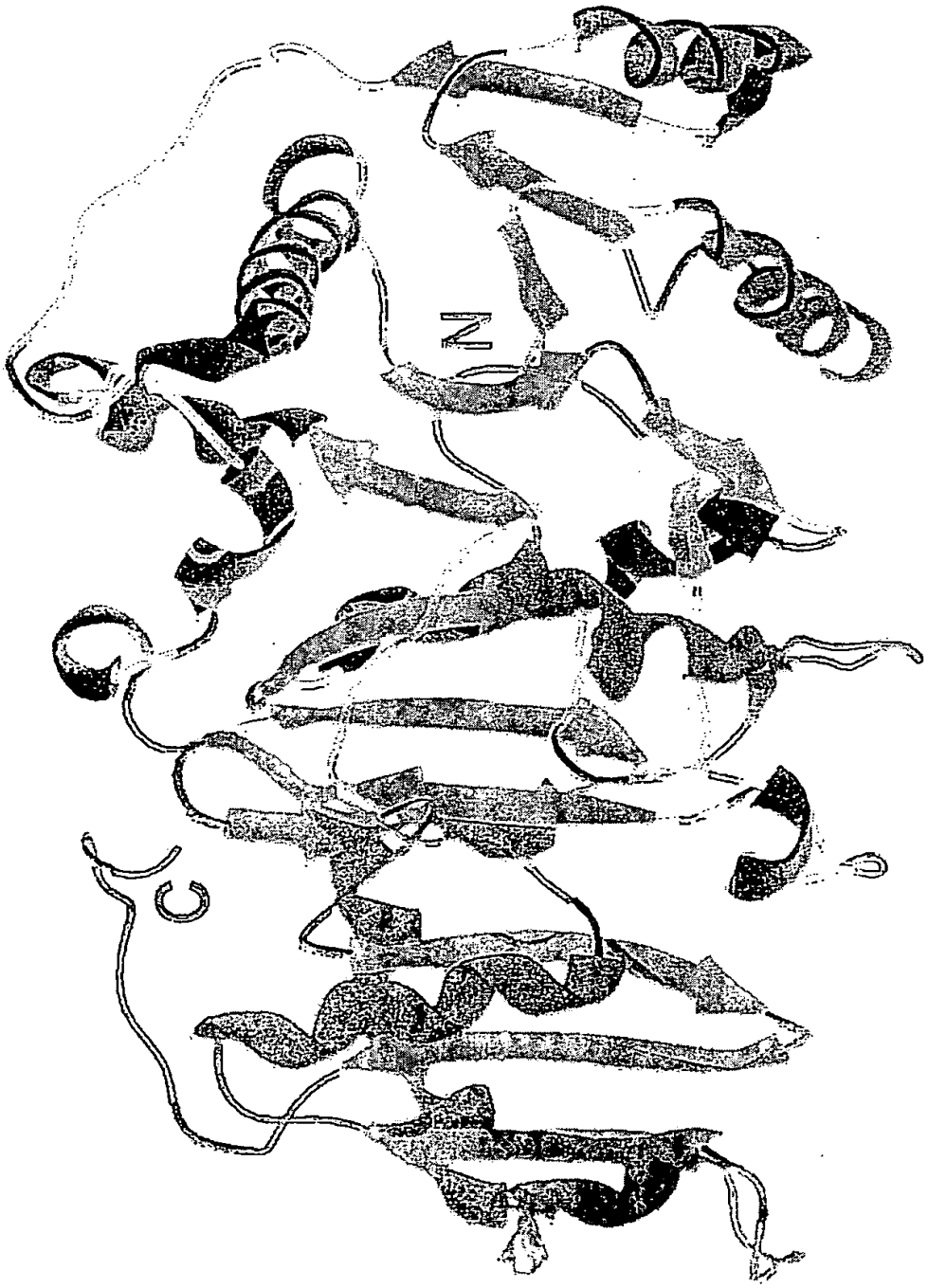
30/53

Figure 20



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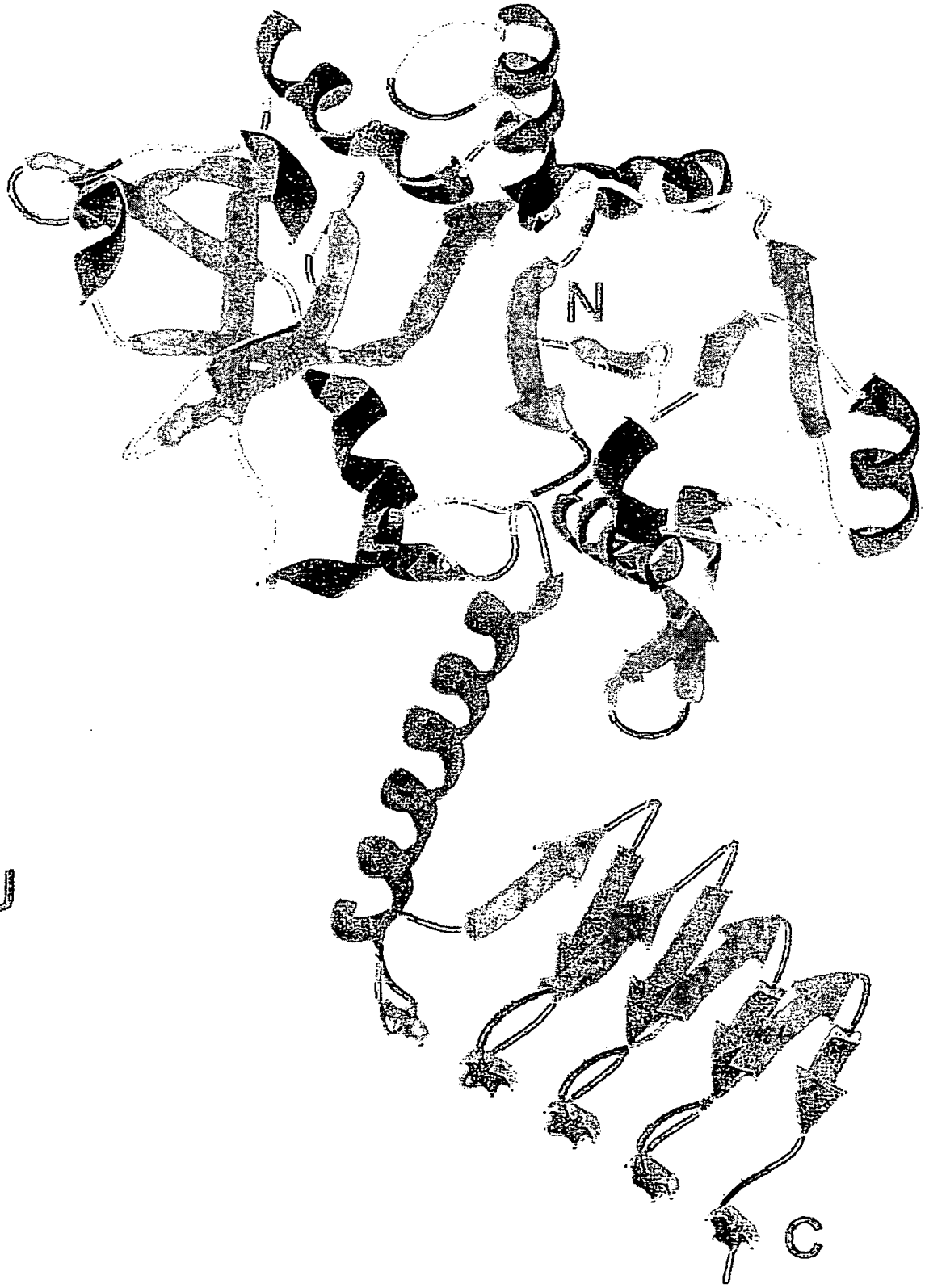
Figure 21



GnTI

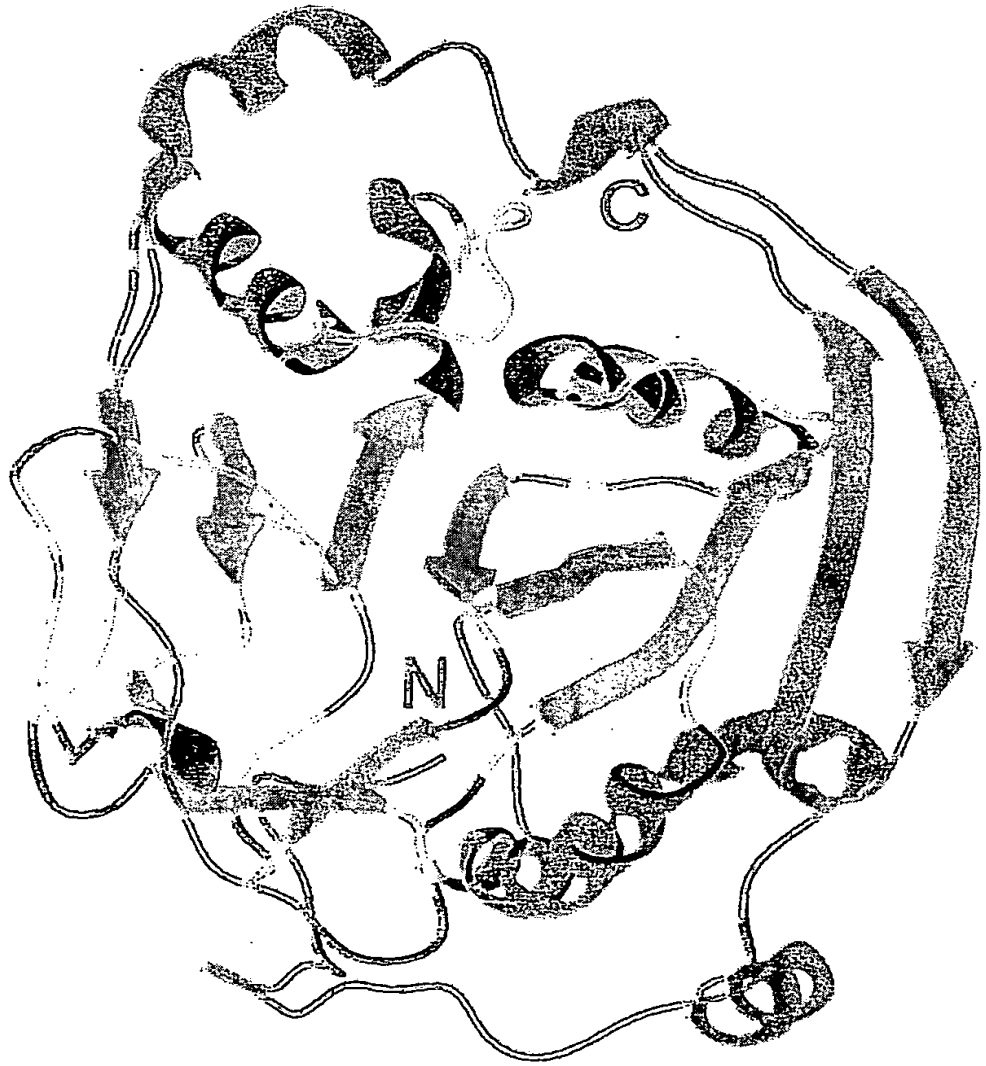
32/53

Figure 22



GlmU

Figure 23



GalT

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Figure 24



SpsA

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Figure 25

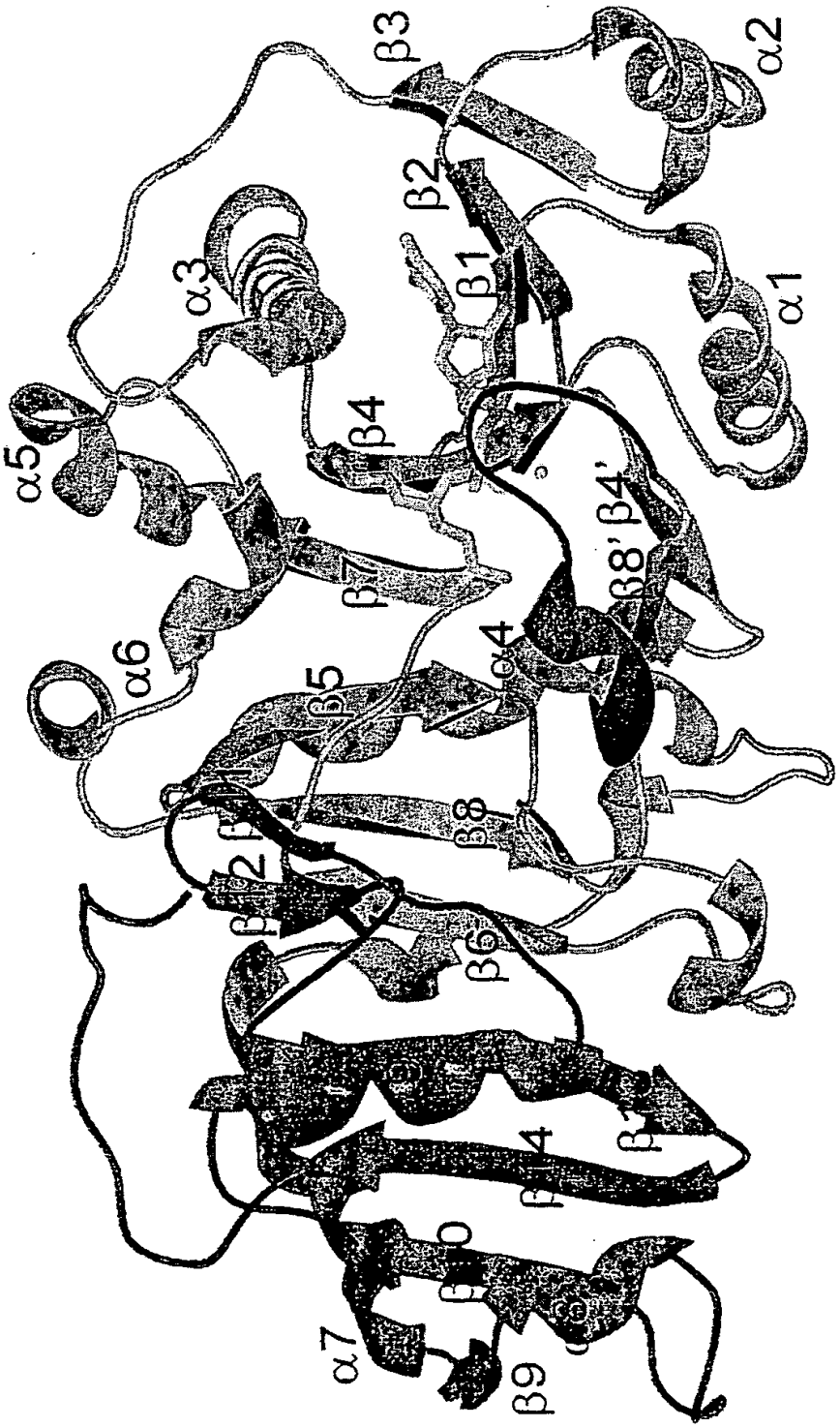
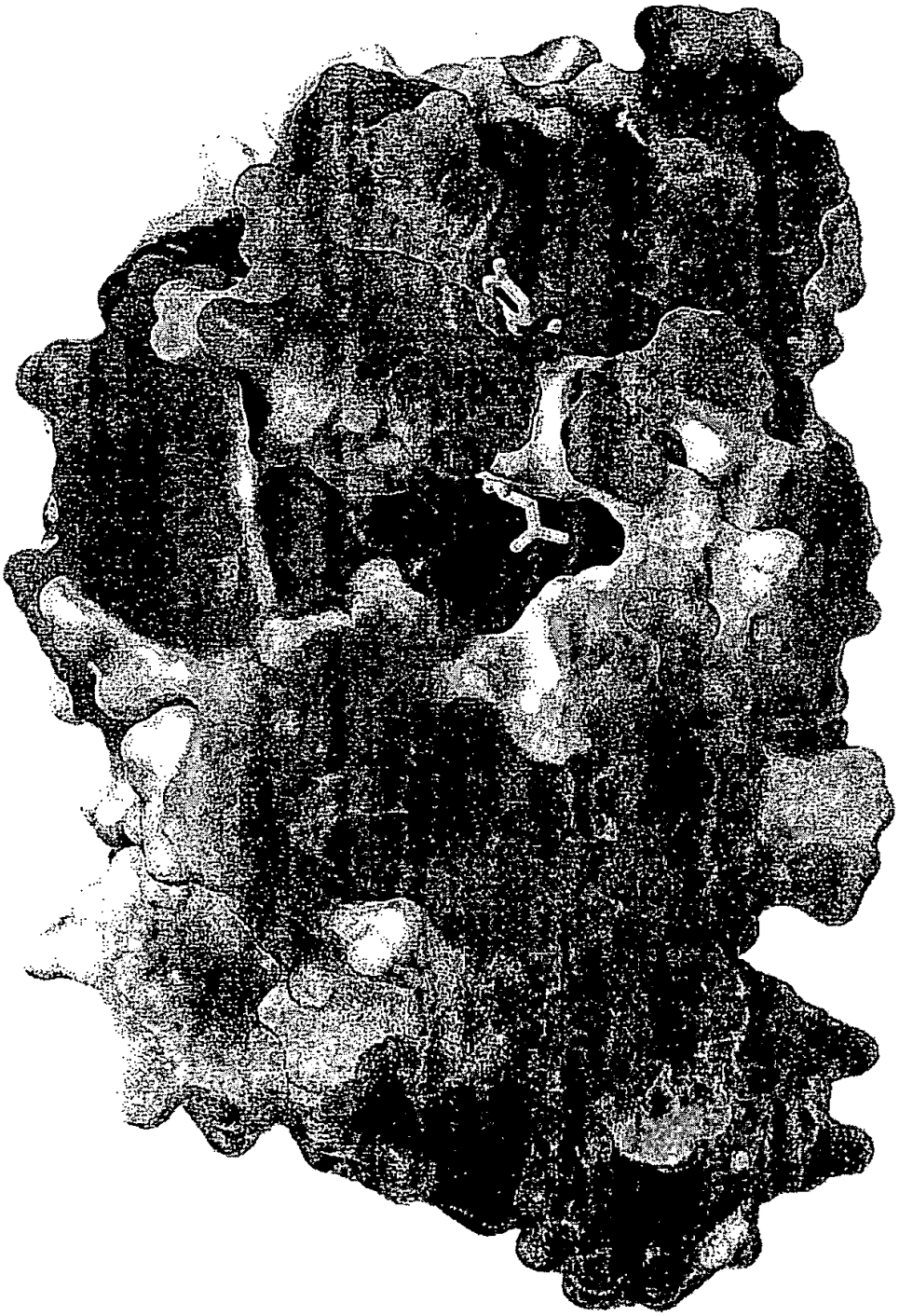


Figure 26



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Figure 27

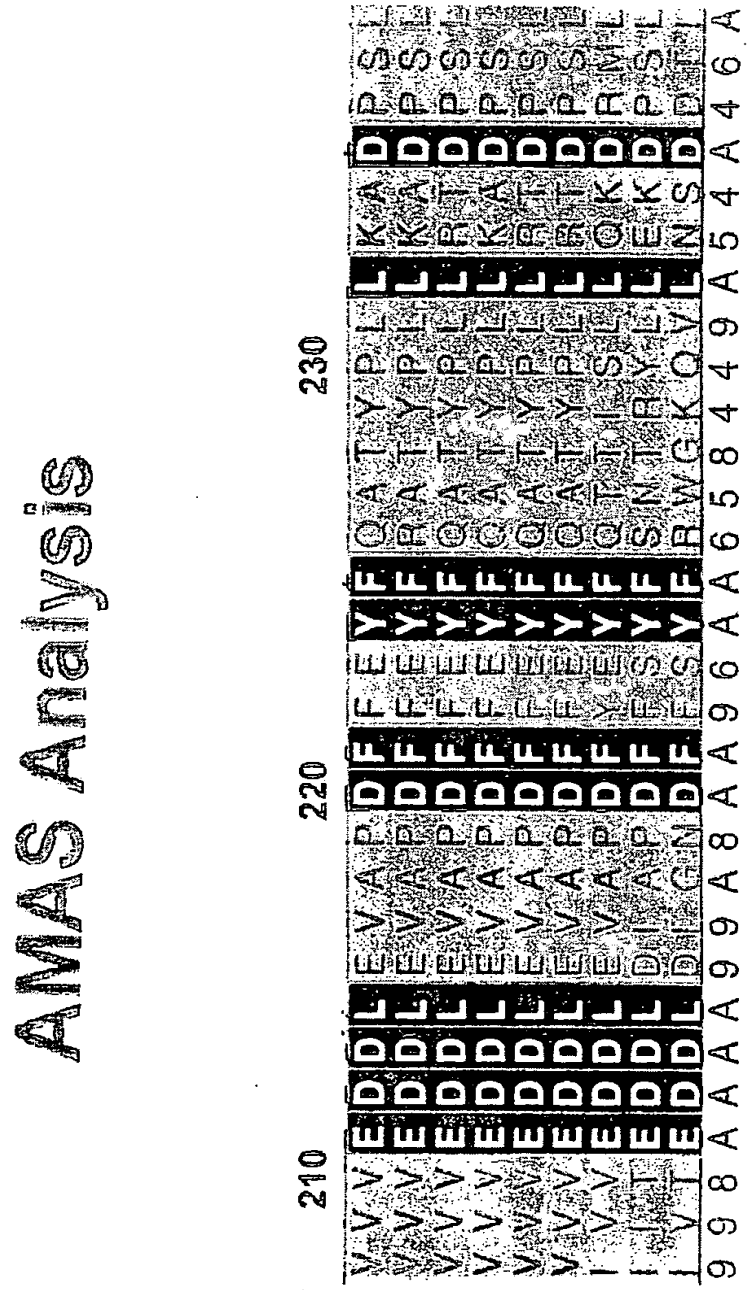


Figure 28

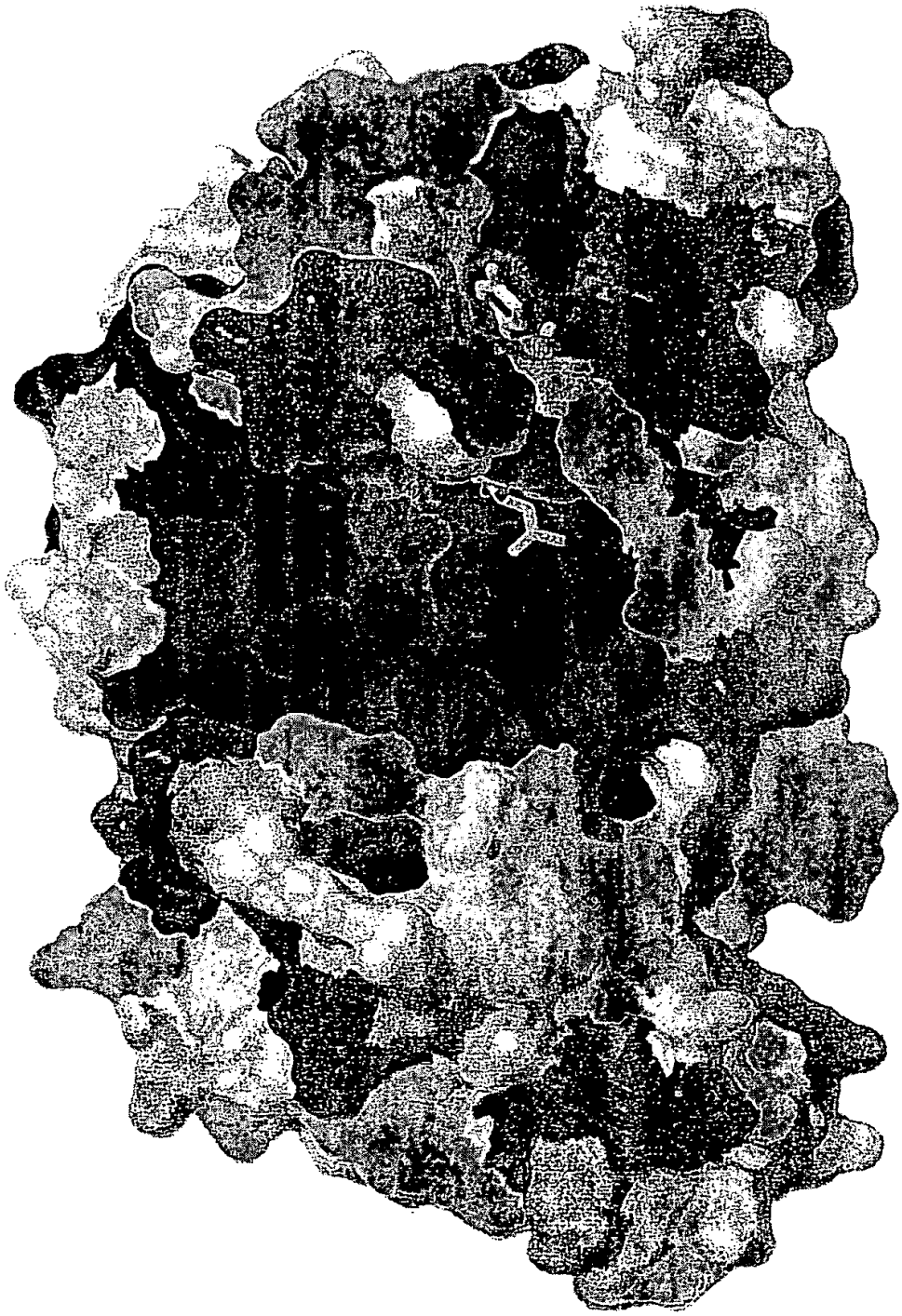


Figure 29



Figure 30

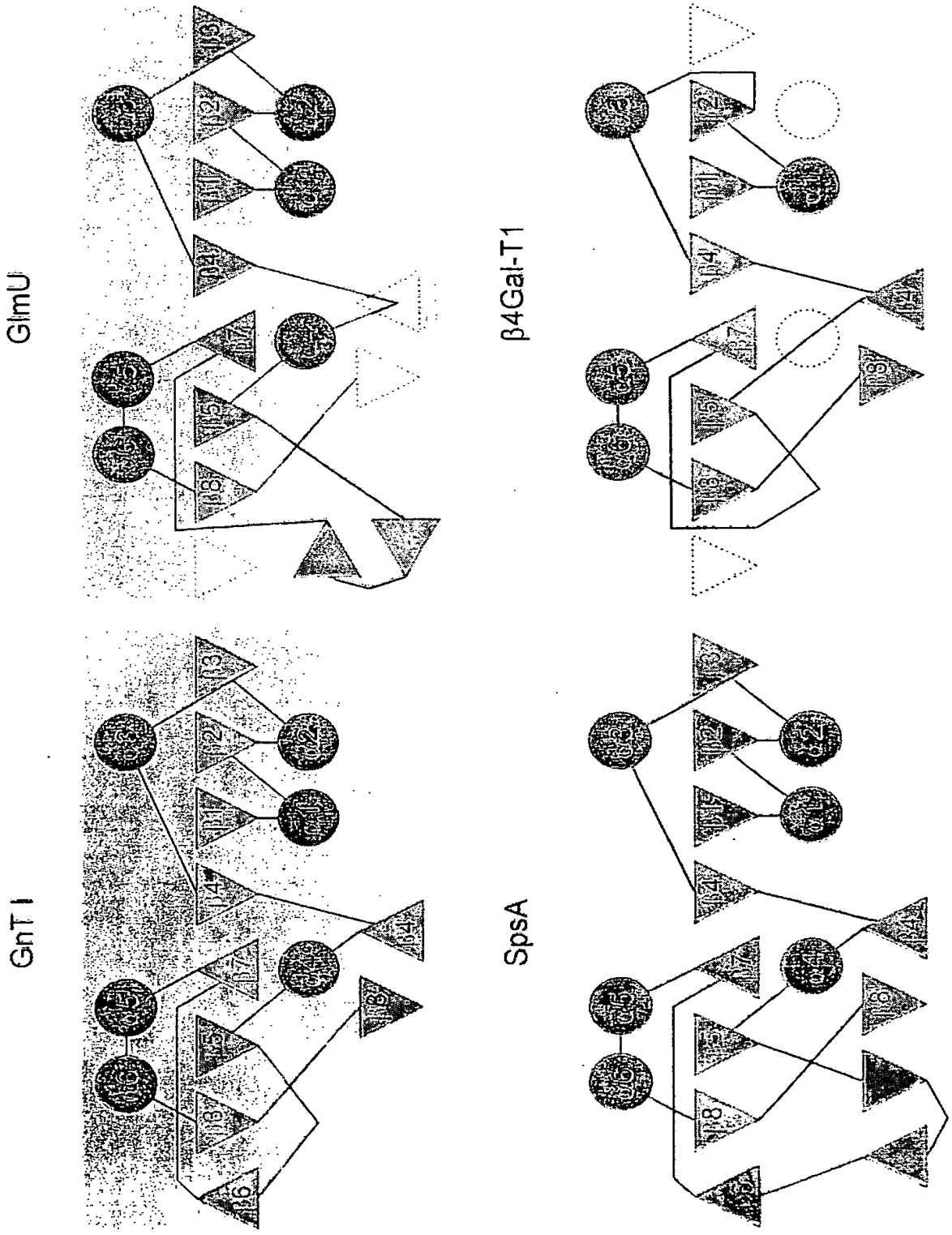


Figure 31

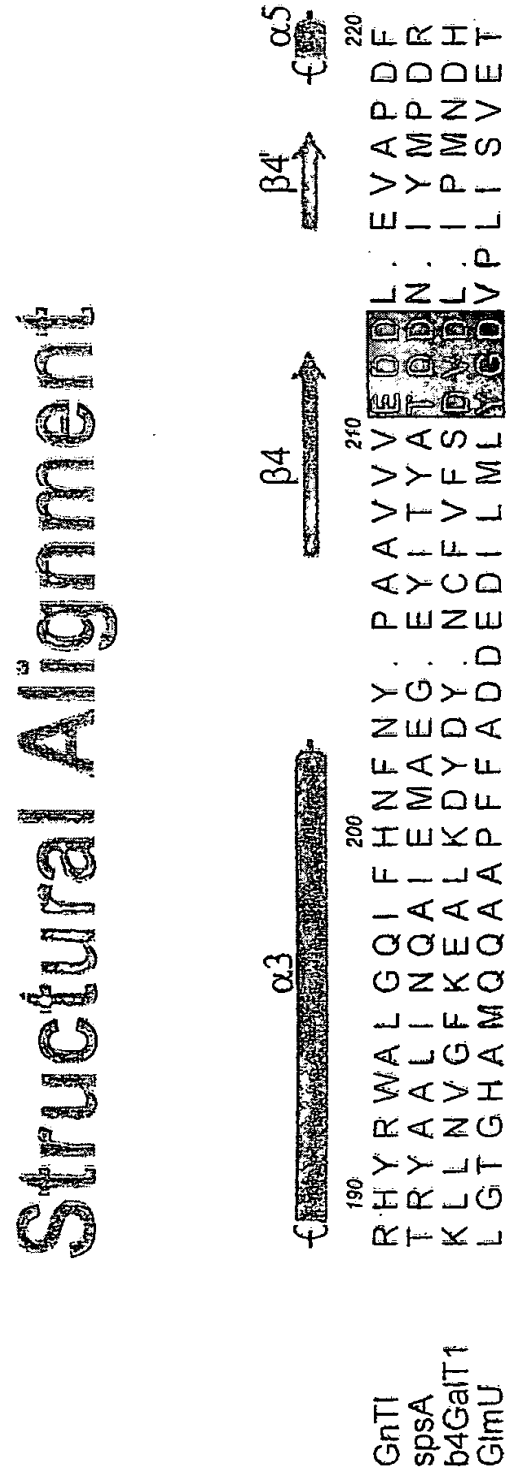

Structural Alignment
α3
β4
β4
α5
α6
β8
GnTI
spsA
b4GalT1
GlmU
190
200
210
220
290
300
310

Figure 32

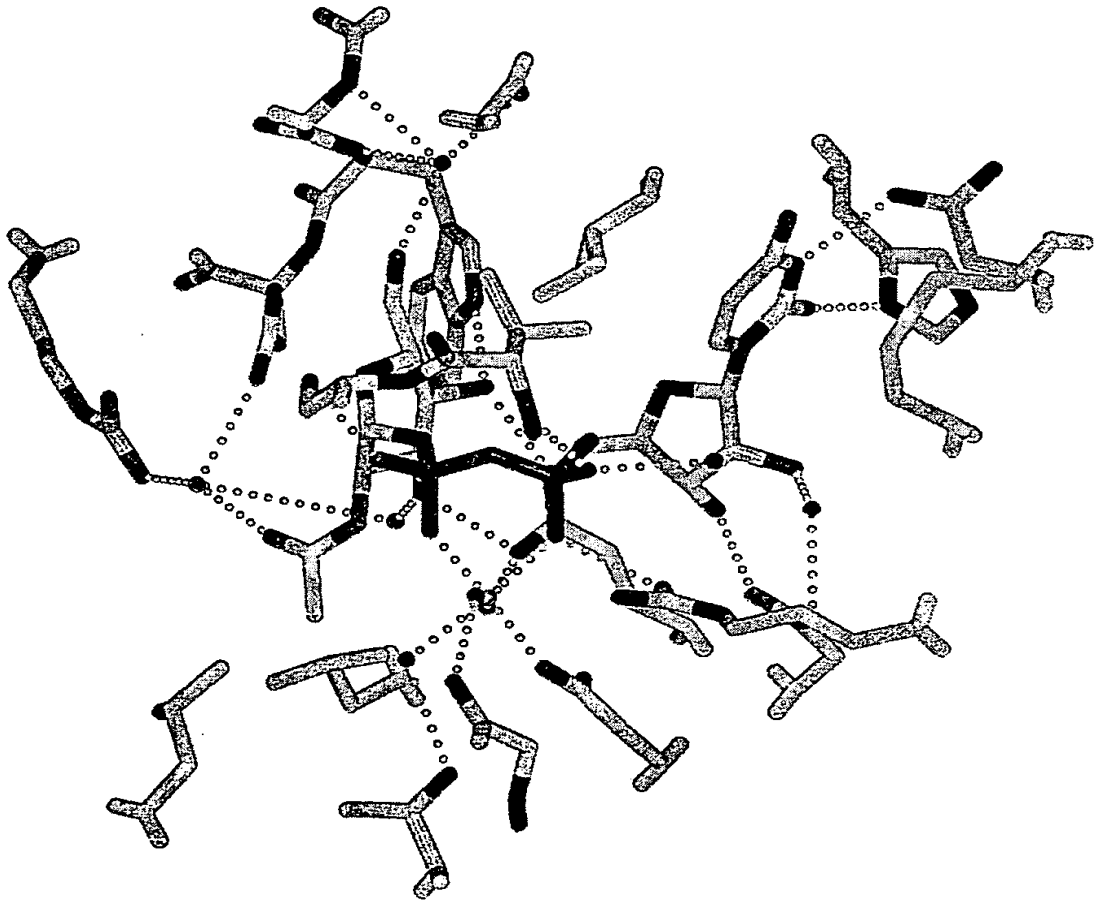


Figure 33A

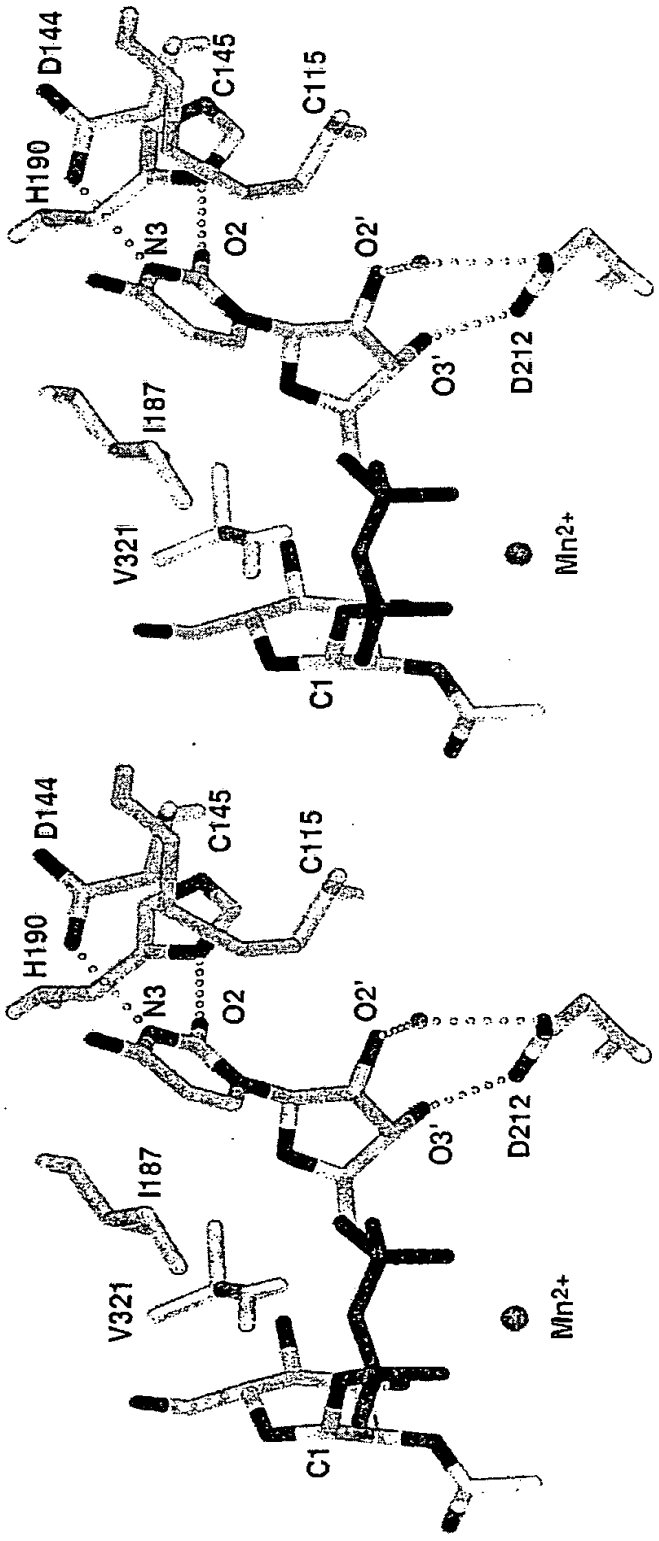

D144
C145
C115
H190
N3
O2
O2'
O3'
D212
I187
V321
Mn2+
C1
D144
C145
C115
H190
N3
O2
O2'
O3'
D212
I187
V321
Mn2+
C1

Figure 33B

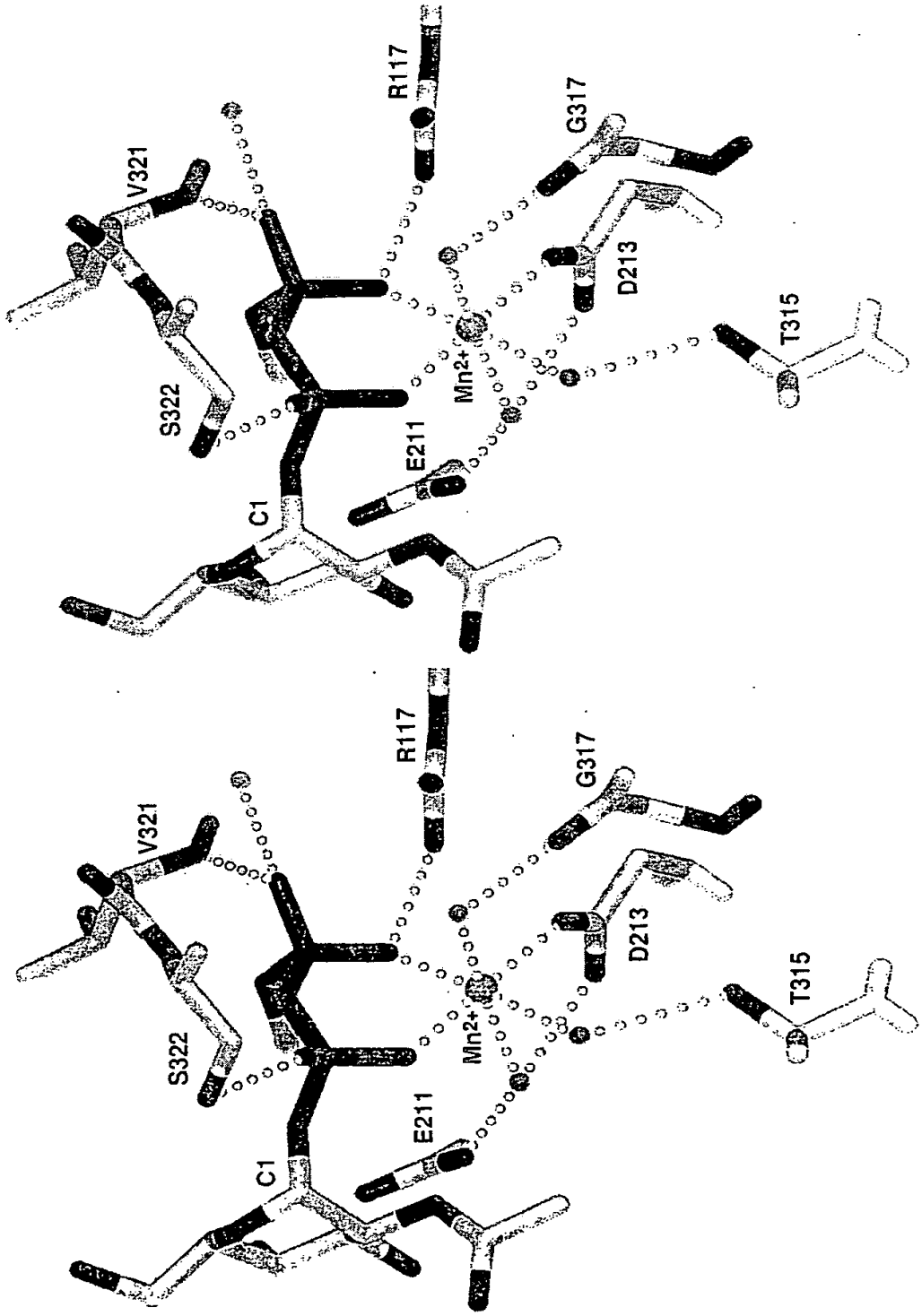

R117
G317
V321
D213
T315
Mn2+
S322
E211
C1
R117
G317
V321
D213
T315
Mn2+
S322
E211
C1

Figure 33C

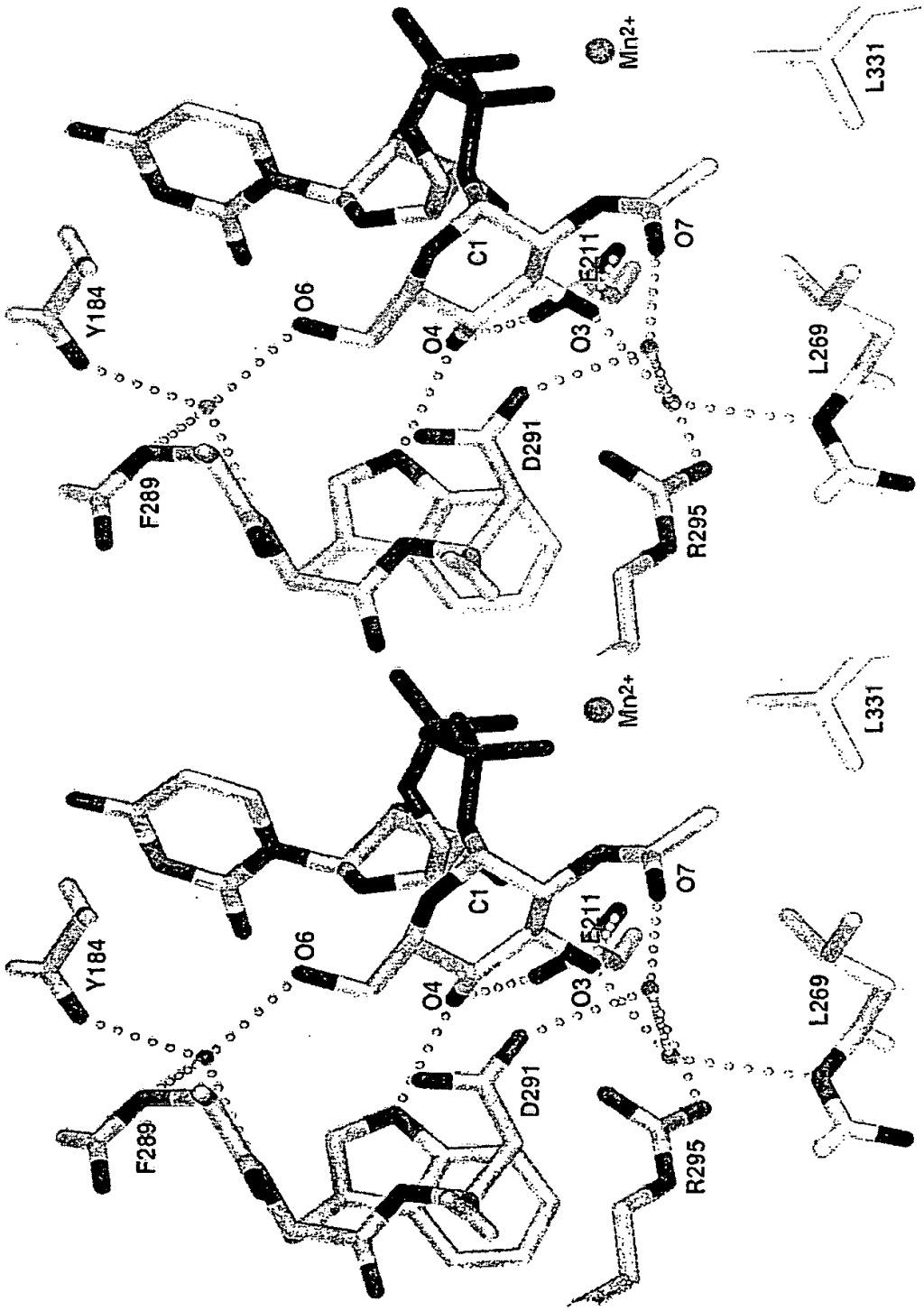
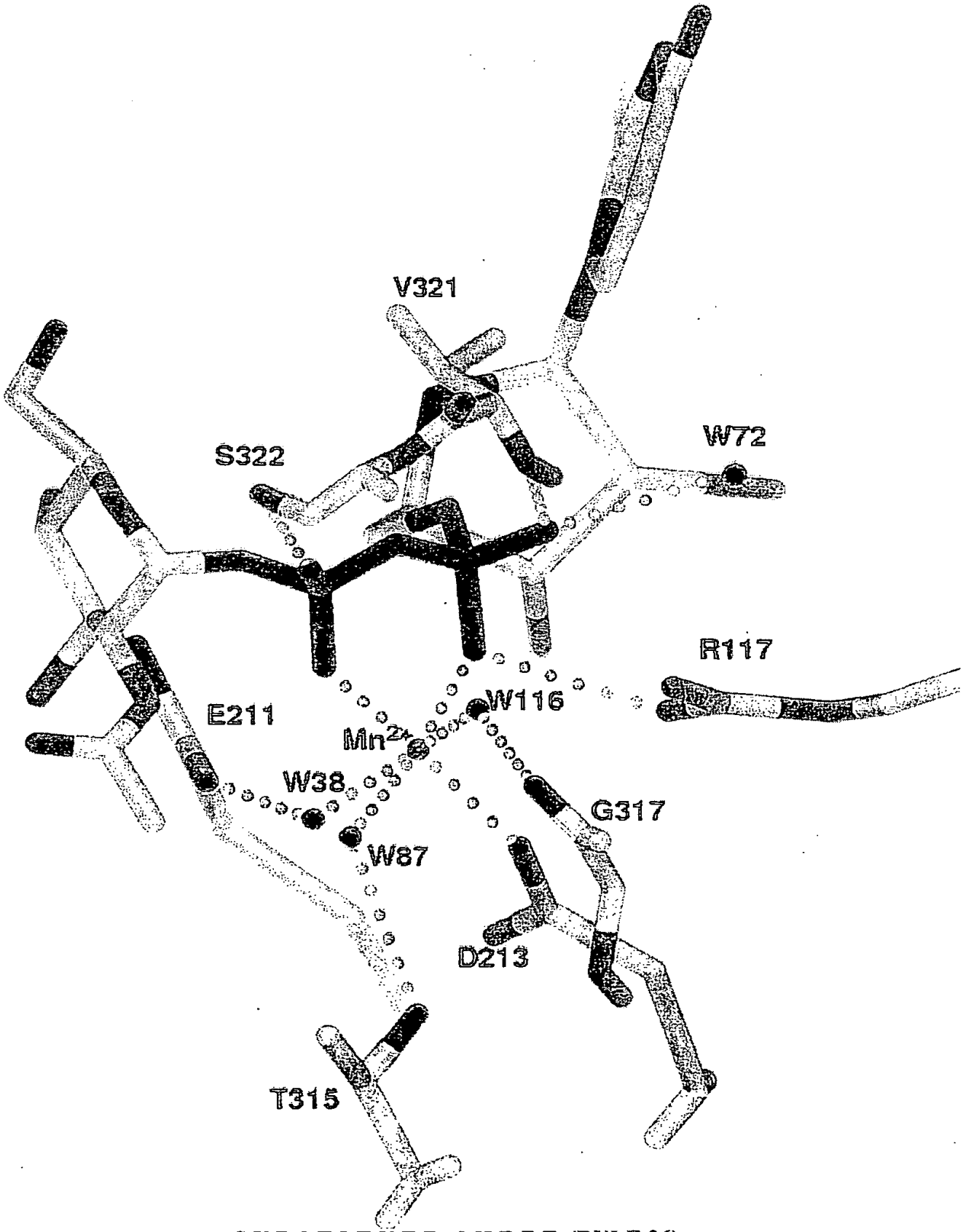

Mn2+
L331
C1
E211
O7
Y184
O6
O4
O3
L269
D291
F289
R295
Mn2+
L331
C1
E211
O7
Y184
O6
O4
O3
L269
D291
F289
R295

Figure 34



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Figure 35

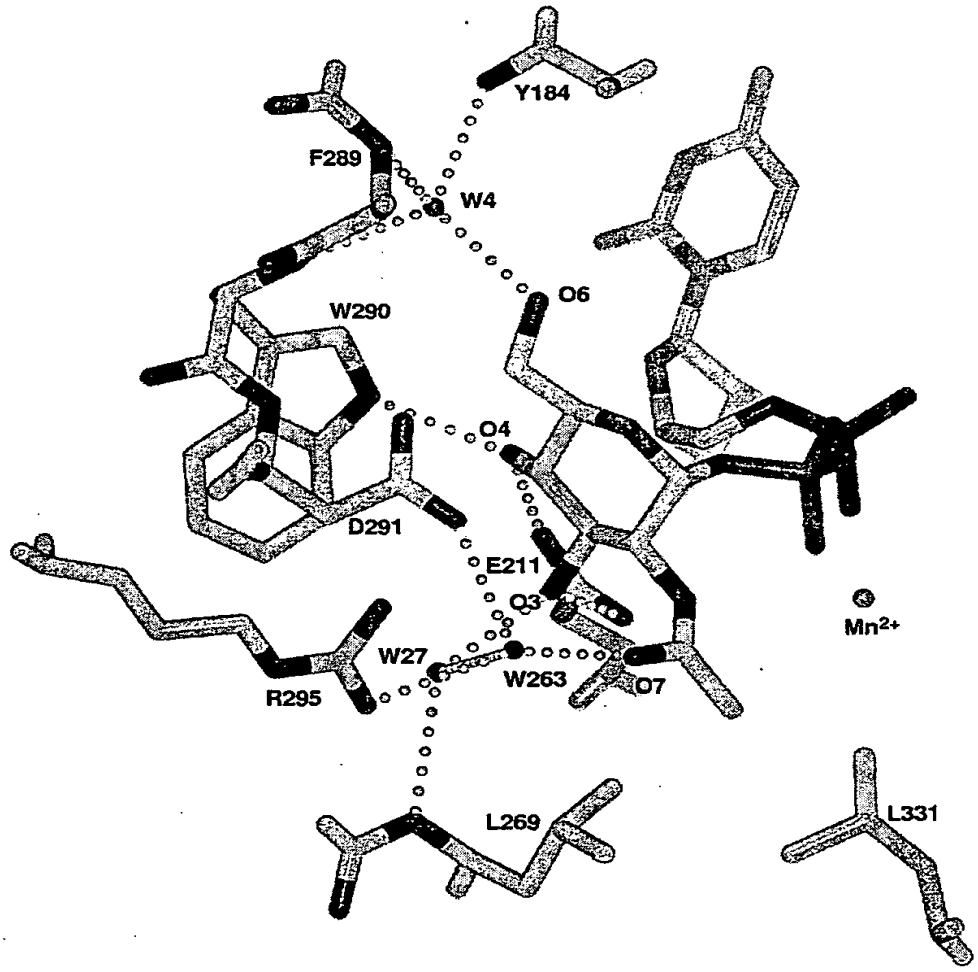


Figure 36

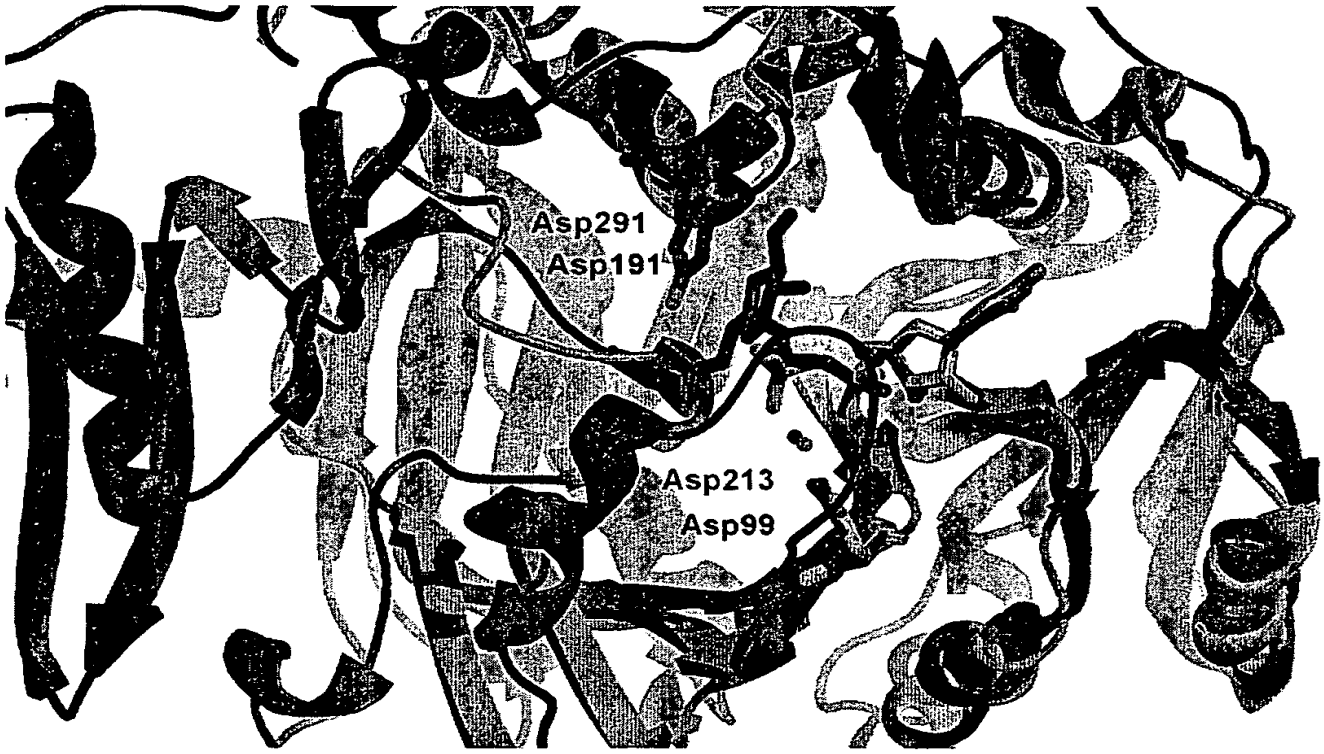


Figure 37

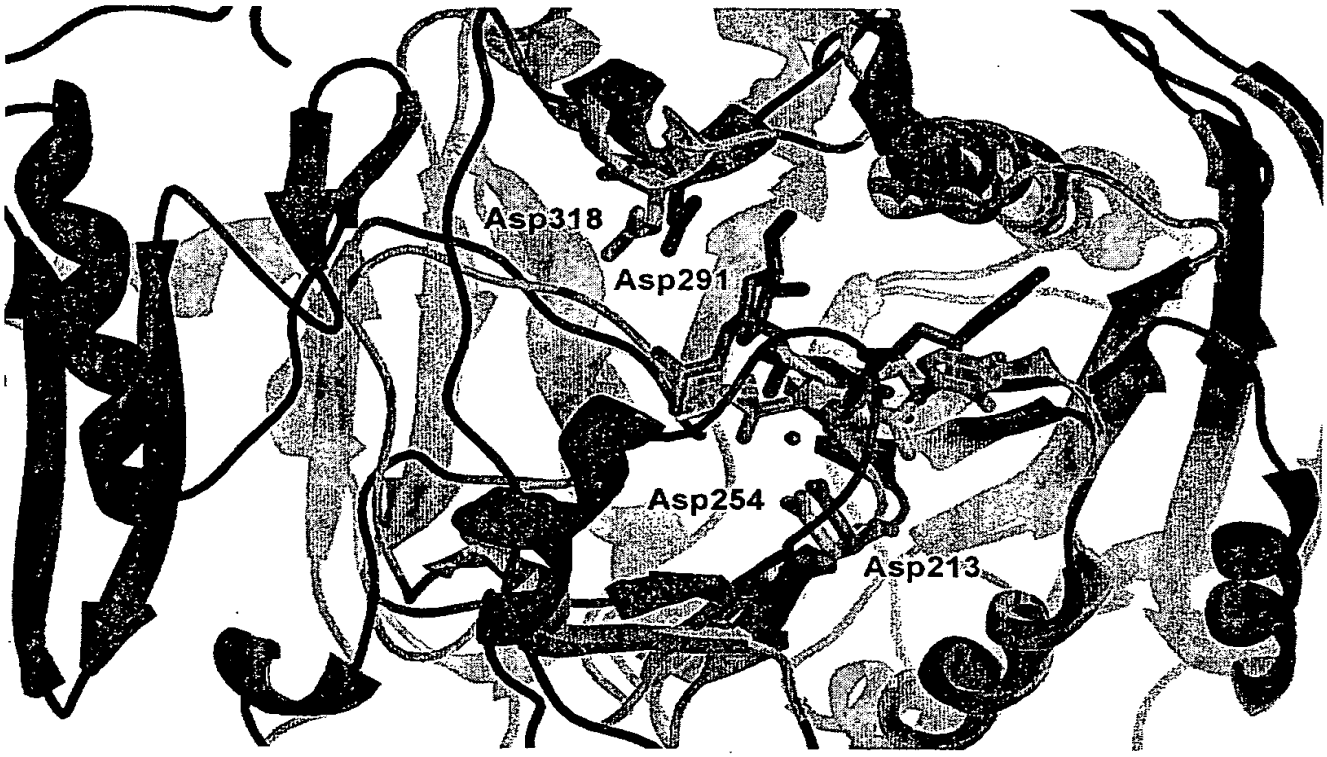


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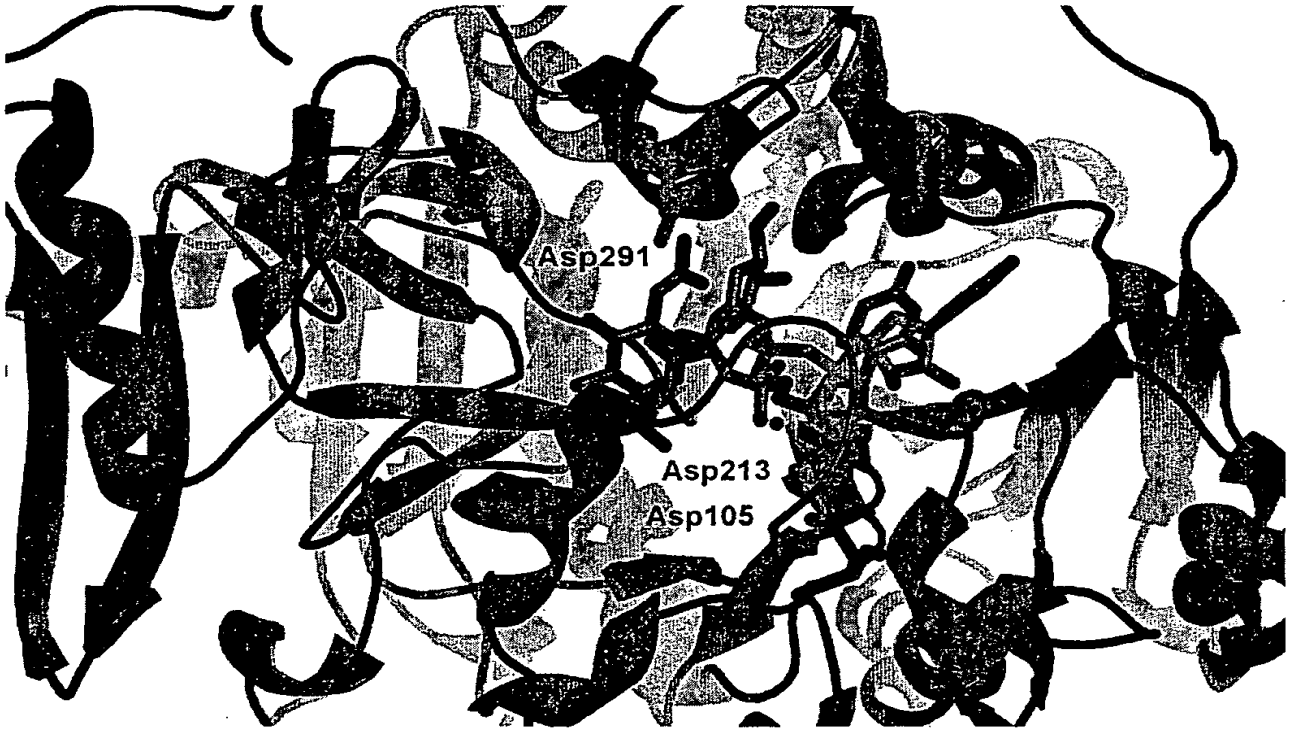


Figure 39

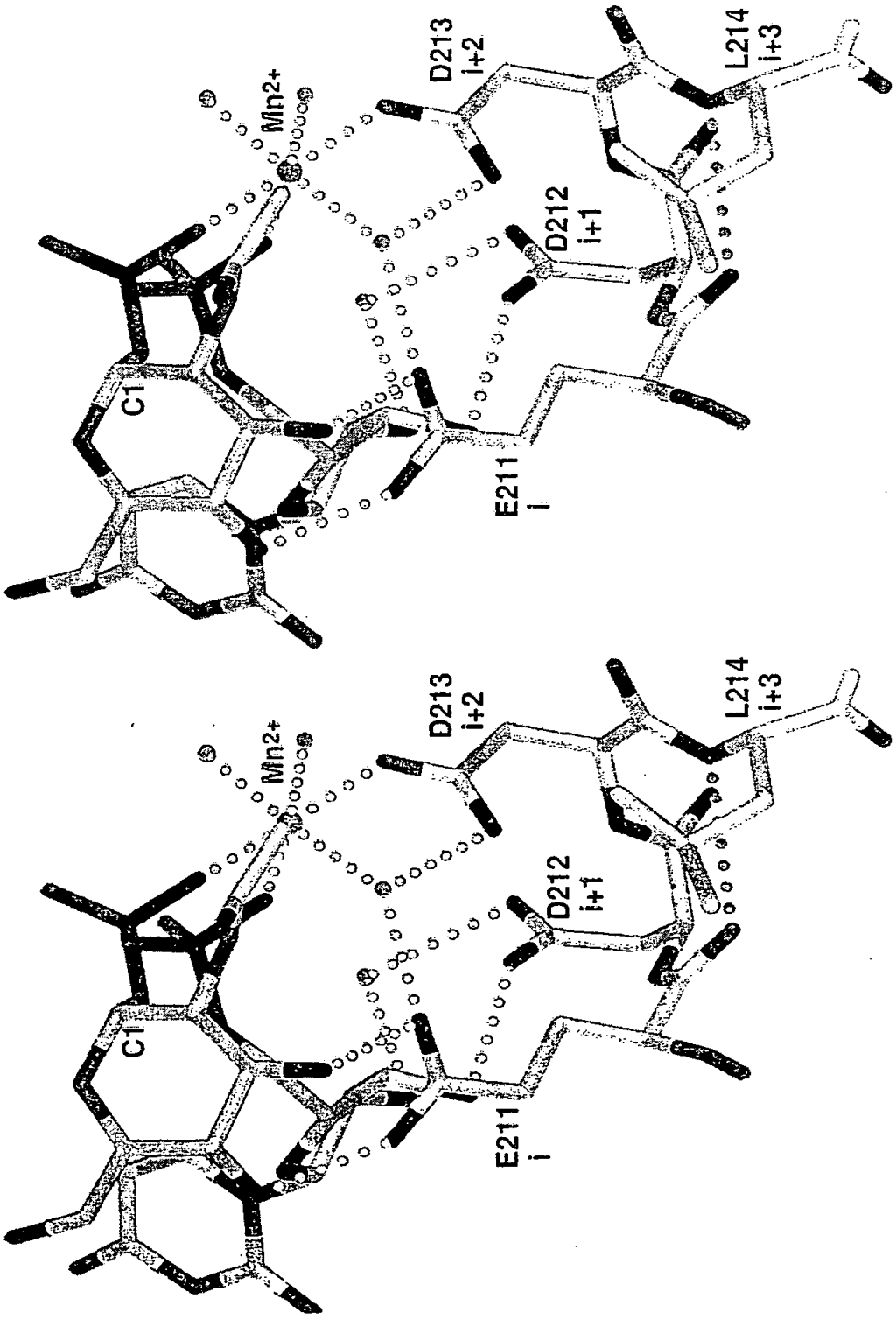

Mn2+
D213
i+2
L214
i+3
D212
i+1
C1
E211
i
Mn2+
D213
i+2
L214
i+3
D212
i+1
C1
E211
i

Figure 40A

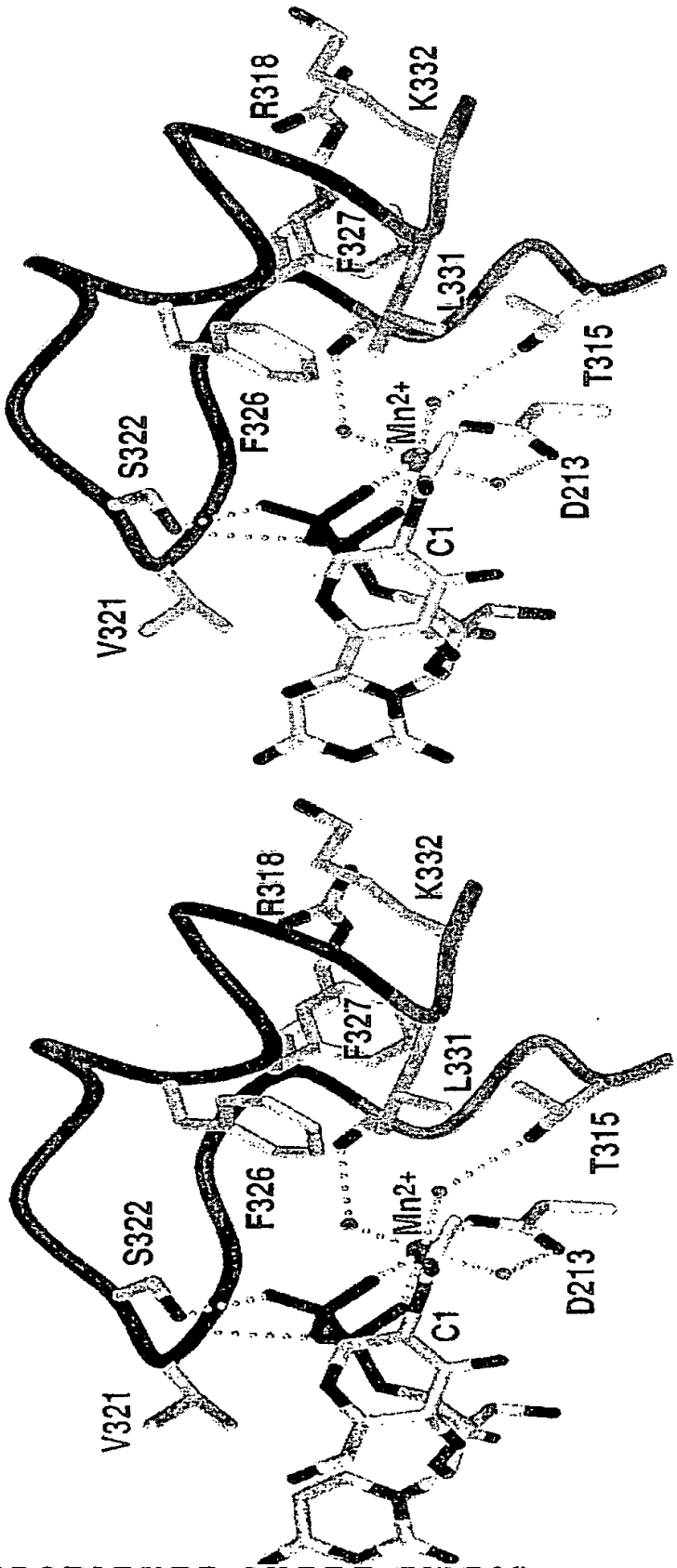
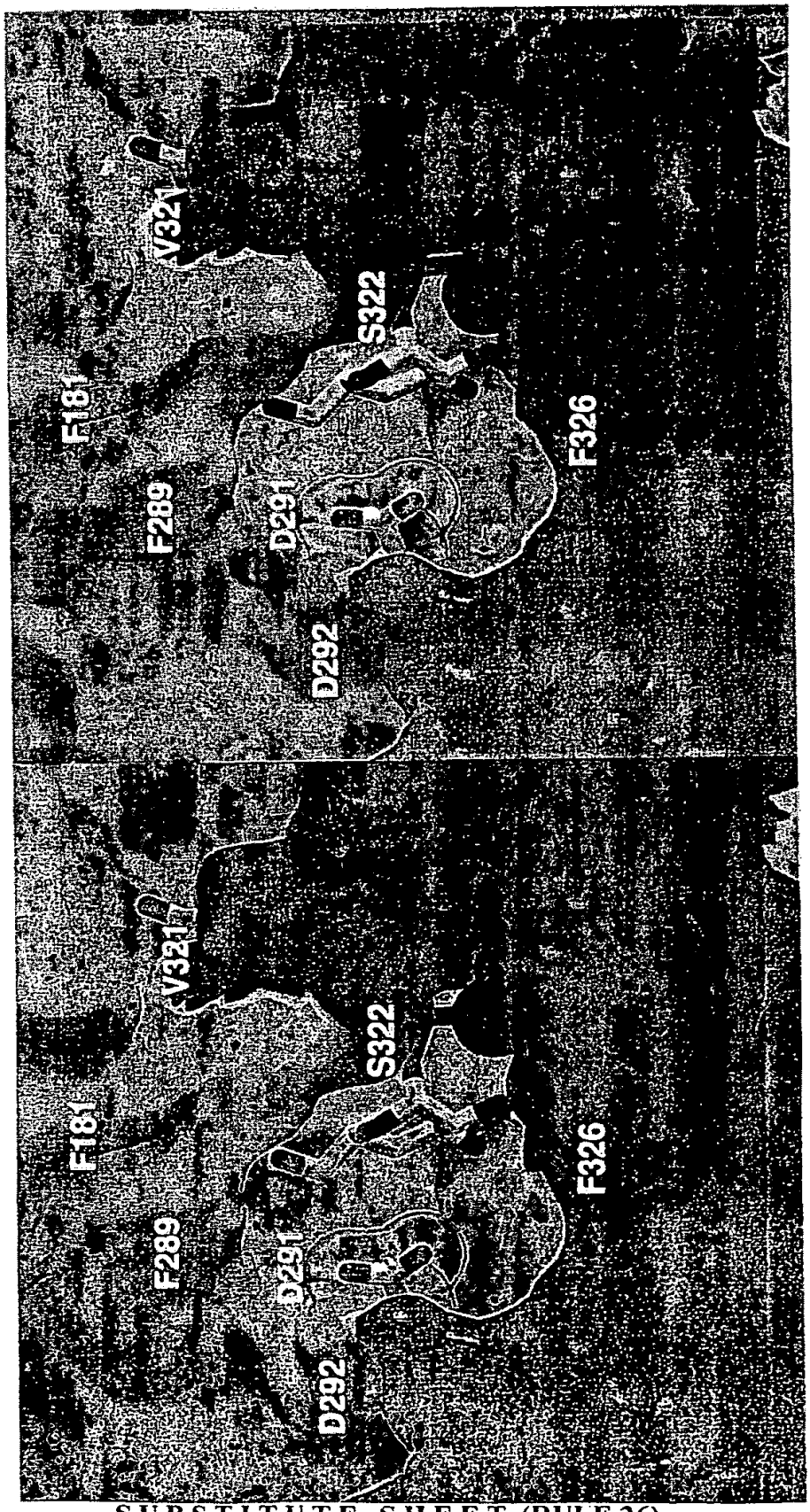

R318
K332
F327
L331
T315
F326
Mn2+
S322
D213
C1
V321
R318
K332
F327
L331
T315
F326
Mn2+
S322
D213
C1
V321

Figure 40B


V321
S322
F181
F289
D291
D292
F326
V321
S322
F181
F289
D291
D292
F326

Sequence Listing

SEQ ID NO 1

VVVEDDLEVAPDFFEYFQATYPLLKADSL

SEQ ID NO 2

VVVEDDLEVAPDFFEYFRATYPLLKADPSL

SEQ ID NO 3

VVVEDDLEVAPDFFEYFQATYPLLRTDPSL

SEQ ID NO 4

IITEDDLDIAPDFFSYFSNTRYLLEKDPSL

SEQ ID NO. 5

IVTEDDLDIGNDFFSYFRWGKQVLNSDDTI

SEQ ID NO 6

RHYRWALGQIFHNFNYPAAVVVEDDLEVAPDFKAFWDDWMRRPEQRKGRACVRPEI

SEQ ID NO 7

TRYAALINQAIEMAEGEYITYATDDNIYMPDRYRIGDARFFWRVNHFYPFYPLDE

SEQ ID NO 8

KLLNVGFKEALKDYDYNCFVFSDVDLIPMNDHWGGEDDDIYNRLAFRGMSVSRPNA

SEQ ID NO 9

LGTGHAMQQAAPFFADDEDILMLYGDVPLISVETGEYYITDIIALAYQEGREIVAVHP

INTERNATIONAL SEARCH REPORT

Int. ional Application No
PCT/CA 00/00725

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12N9/10 C12Q1/48 A61K31/70

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
BIOSIS, EPO-Internal

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	CHARNOCK SIMON J ET AL: "Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms." BIOCHEMISTRY, vol. 38, no. 20, 18 May 1999 (1999-05-18), pages 6380-6385, XP002152151 ISSN: 0006-2960	1-3,14, 15,20, 21,27, 29,34,35
Y	the whole document	18,19, 22-26, 28,30-32

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[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
8 November 2000	22/11/2000

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	VAN DER SCHAAL, C

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Form PCT/ISA/210 (second sheet) (July 1992)

INTERNATIONAL SEARCH REPORT

Int. ional Application No
PCT/CA 00/00725

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
X	NISHIKAWA Y ET AL: "CONTROL OF GLYCOPROTEIN SYNTHESIS PURIFICATION AND CHARACTERIZATION OF RABBIT LIVER UDP-N-ACETYLGLUCOSAMINE ALPHA-3-D-MANNOSIDE BETA-1 2-N ACETYLGLUCOSAMINYLTRANSFERASE I" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 263, no. 17, 1988, pages 8270-8281, XP002152152 ISSN: 0021-9258	1-17,20, 21,27, 29,34,35
Y	the whole document	18,19, 22-26, 28,30-32
X	ULLMAN C AND PERKINS S: "A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities" BIOCHEMICAL JOURNAL, vol. 326, 1997, pages 929-941, XP002152153 page 937, paragraph 1	1-17,20, 21,27, 29,34,35
Y	DATABASE BIOSIS 'Online! BIOSCIENCES INFORMATION SERVICE, PHILADELPHIA, PA, US; 1994 SARKAR MOHAN: "Expression of recombinant rabbit UDP-GlcNAc:alpha-3-D-mannoside beta-1,2-N-acetylglucosaminyltransferase I catalytic domain in Sf9 insect cells." Database accession no. PREV199598004969 XP002152154 abstract & GLYCOCONJUGATE JOURNAL, vol. 11, no. 3, 1994, pages 204-209, ISSN: 0282-0080	18,19
Y	KUNTZ I D ET AL: "STRUCTURE-BASED MOLECULAR DESIGN" ACCOUNTS OF CHEMICAL RESEARCH,US,AMERICAN CHEMICAL SOCIETY. WASHINGTON, vol. 27, no. 5, May 1994 (1994-05), pages 117-123, XP000885741 ISSN: 0001-4842 cited in the application the whole document	20, 22-26, 28,30-33
Y	GSCHWEND D A ET AL: "MOLECULAR DOCKING TOWARDS DRUG DISCOVERY" JOURNAL OF MOLECULAR RECOGNITION,GB,HEYDEN & SON LTD., LONDON, vol. 9, 1996, pages 175-186, XP000882526 ISSN: 0952-3499 the whole document	20, 22-26, 28,30-33

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FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Although claim 31 is directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound/composition.

Although claims 34 and 35 could be considered as a mere presentation of information, Rule 39.1 (v and vi) PCT, the search has been carried out as far as possible in our systematic documentation

Continuation of Box I.2

Present claims 20 27 29 -32 relate to compounds defined by reference to a desirable characteristic or property, namely modulating glycosyltransferases
The claims cover all compounds having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for only UDP-GlcNAc. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the compound by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, the search has been carried out for those parts of the claims which appear to be clear, supported and disclosed, namely those parts relating to the UDP-GlcNAc.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.